



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:22 AM UTC

PDB ID : 6ZHA / pdb_00006zha
EMDB ID : EMD-11217
Title : Cryo-EM structure of DNA-PK monomer
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-21
Resolution : 3.91 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

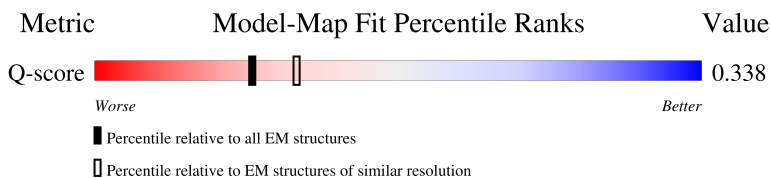
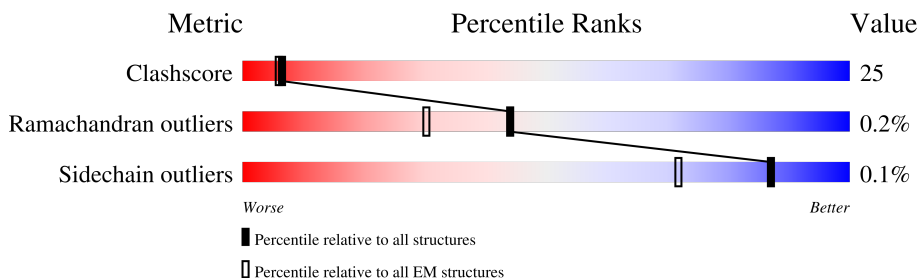
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7920 (3.41 - 4.41)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4156	
2	B	609	
3	C	732	
4	D	25	

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Mol	Chain	Length	Quality of chain
5	E	24	 12% 88%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38289 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3707	Total	C	N	O	S	0	0
			29124	18685	4920	5334	185		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	489	Total	C	N	O	S	0	0
			3908	2504	663	723	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	539	Total	C	N	O	S	0	0
			4260	2733	717	787	23		

- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	25	Total	C	N	O	P	0	0
			510	248	94	144	24		

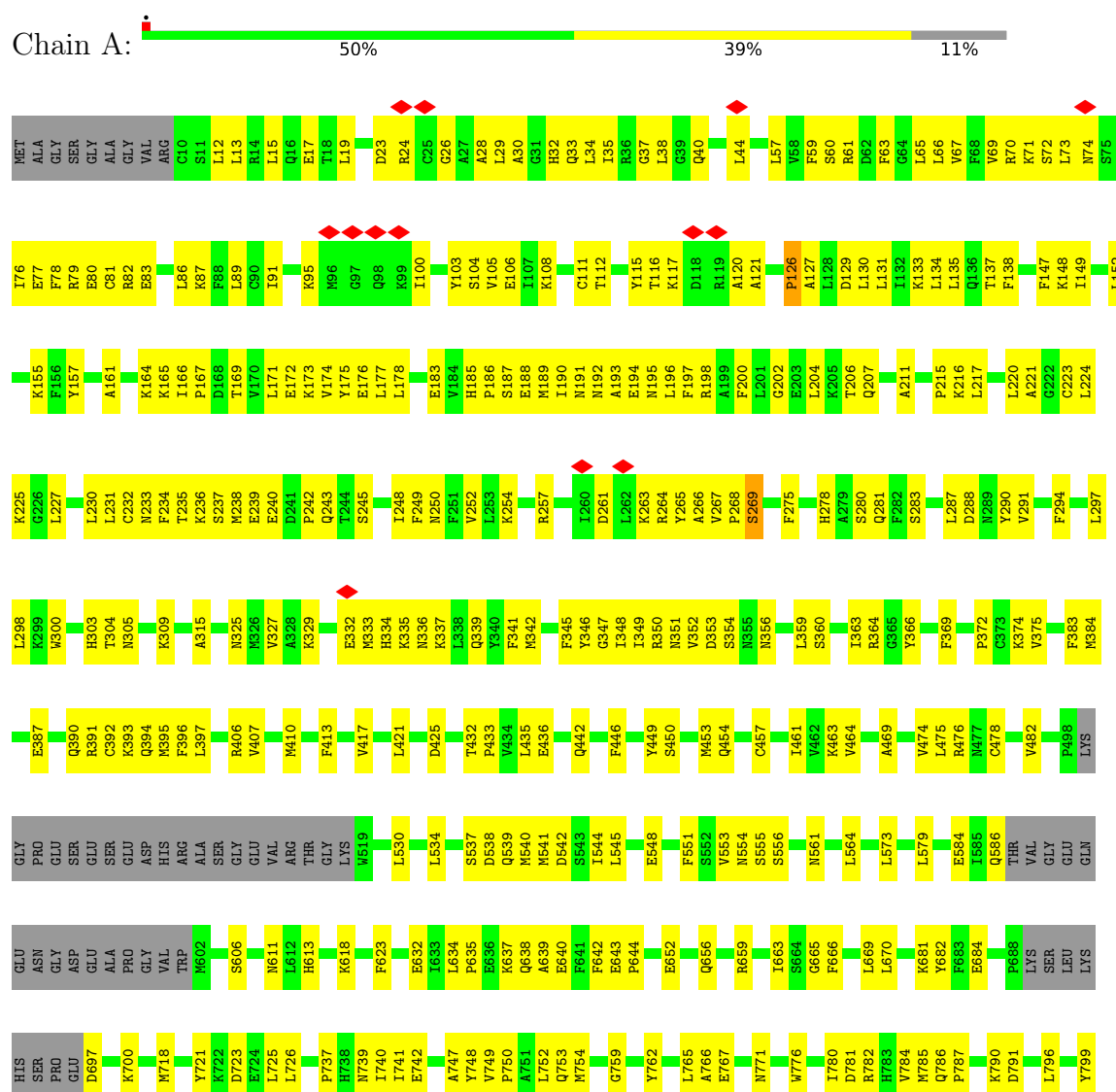
- Molecule 5 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	24	Total	C	N	O	P	0	0
			487	240	80	145	22		

3 Residue-property plots

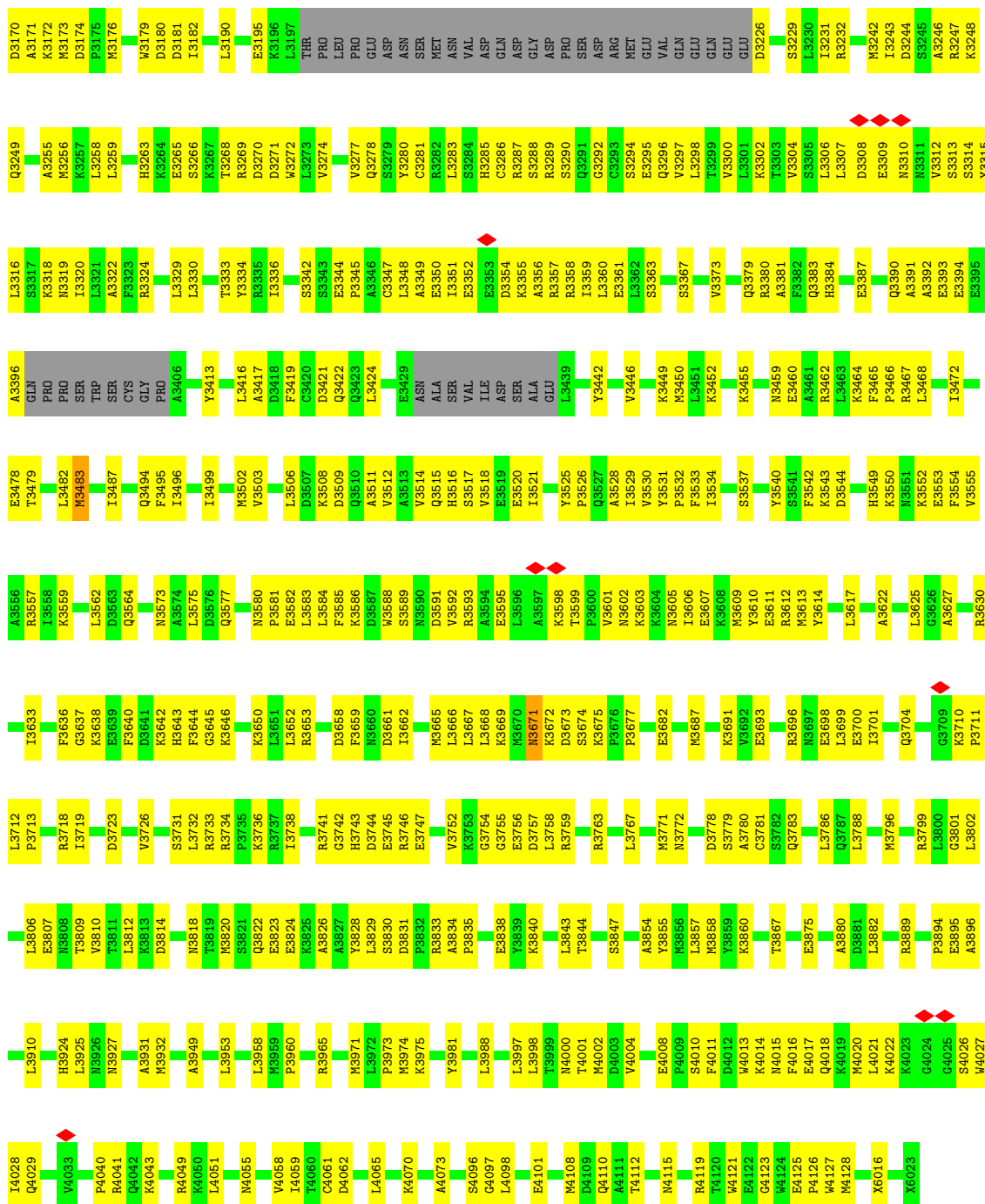
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-dependent protein kinase catalytic subunit,DNA-PKcs



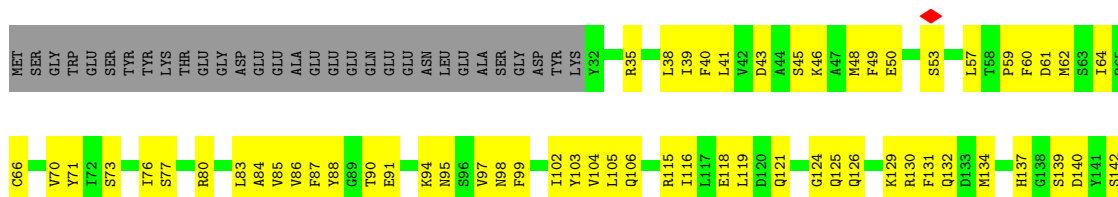
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T1856	A1786	L1710	K1628	LEU	G1462	G1383	M1303	V1211	I1137	E1050	GLN	K801
K1857	R1787	R1711	C1629	SER	G1462	G1383	H1304	K1212	K1140	N1055	ALA	S802
E1860	C1791	R1712	W1632	SER	I1467	F1384	D1305	E1214	K1141	S1058	P956	S803
F1863	Q1794	V1713	W1633	GLN	W1633	I1386	I1306	E1215	H1142	L1059	W958	A804
Q1794	Q1794	Q1716	D1636	GLY	Q1471	G1387	I1307	G1216	V1143	F1060	P957	LEU
V1795	V1795	L1717	S1472	S1549	S1472	A1308	A1368	V1217	M1146	K1061	Y959	
L1798	L1798	L1719	T1473	H1552	T1473	A1309	E1309	S1218	K1147	Y962		
E1799	E1799	F1640	D1474	F1553	D1474	V1389	E1310	F1219	K1148	L1066	R963	THR
K1869	S1800	H1721	E1640			I1391	K1311	L1220	A1148	L1066	R964	LYS
K1870	K1870	F1722	M1643	E1557	H1477	Q1390	C1312	I1221	K1149	H1069	R964	ASN
M1871	E1803	P1723	W1479	Y1558	S1478	H1392	F1313	N1222	K1150	P1070	T965	ASN
G1872	H1804	M1724	V1479		V1479	A1393	G1314	T1223	R1151	P1070	R966	TRP
Y1873	Y1873	Q1725	L1483	L1562	E1482	H1394	THR	F1224	R1152	N1071	P967	GLU
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L1877	D1808	S1726	A1650	T1566	S1484	H1395	ALA	G1226	P1154	F1073	R971	ALA
D1878	F1810	E1728	K1651	I1567	S1485	P1396	ALA	G1234	R1155	R1075	R971	LEU
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S1882	T1815	F1736	G1494	L1572	G1494	K1412	S1323	L1244	S1162	F1082	ALA	LYS
R1883	R1816	S1664	D1495	K1573	D1495	D1413	Q1325	R1245	L1163	I1085	R981	GLY
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K1895	K1745	V1671	L1503	L1582	R1420	R1420	V1337	L1257	L1173	L1095	W994	HIS
T1896	Y1751	T1673	D1504	M1583	E1421	E1421	V1338	L1257	C1176	V1096	A921	LEU
N1897	Q1754	I1676	S1506	S1586	T1424	T1424	R1340	L1260	E1097	E1097	K999	LYS
V1898	R1828	S1677	C1507	L1587	A1425	A1425	C1340	L1261	Q1180	Q1098	Q1004	LYS
F1900	H1830	L1678	K1508	M1589	Q1426	Q1426	Y1341	L1261	T1181	F1099	D1005	THR
H1901	L1758	D1681	Q1509		I1428	I1428	S1352	L1264	H1185	E1102	T1006	ASN
S1902	L1759	T1692	L1514		E1429	E1429	P1353	E1265	K1186	E1102	V1007	LEU
S1903	M1762	K1683	A1518	M1592	E1429	E1429	W1356	G1266	K1186	V1105	A1008	SER
C1904	T1763	L1684	A1519	V1593	A1518	A1518	L1359	Y1267	L1190	I1106	L1009	SER
I1905	E1764	D1685	A1520	V1596	A1520	A1520	L1360	Y1267	Y1192	Y1107	E1011	ASN
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E1907	E1838	H1687	L1524		L1524	P1439	D1362	T1275	P1196	L1113	I1013	A845
F1839	F1839	L1688	G1525	S1604	G1525	Q1442	C1364	T1275	L1197	L1114	L1014	I946
F1840	F1840	K1689	E1526		E1526	Q1442	C1364	A1278	L1198	H1115	V1018	L948
N1909	E1769	G1690	R1527	K1617	R1527	V1443	T1366	A1278	L1198	P1199	M941	E949
E1910	T1842	Q1691	L1528	L1618	L1528	D1444	L1367	L1282	E1118	E1118	L942	E850
T1912	I1843	A1692		A1619		R1445	L1367	L1282	K1119	K1119	G943	I851
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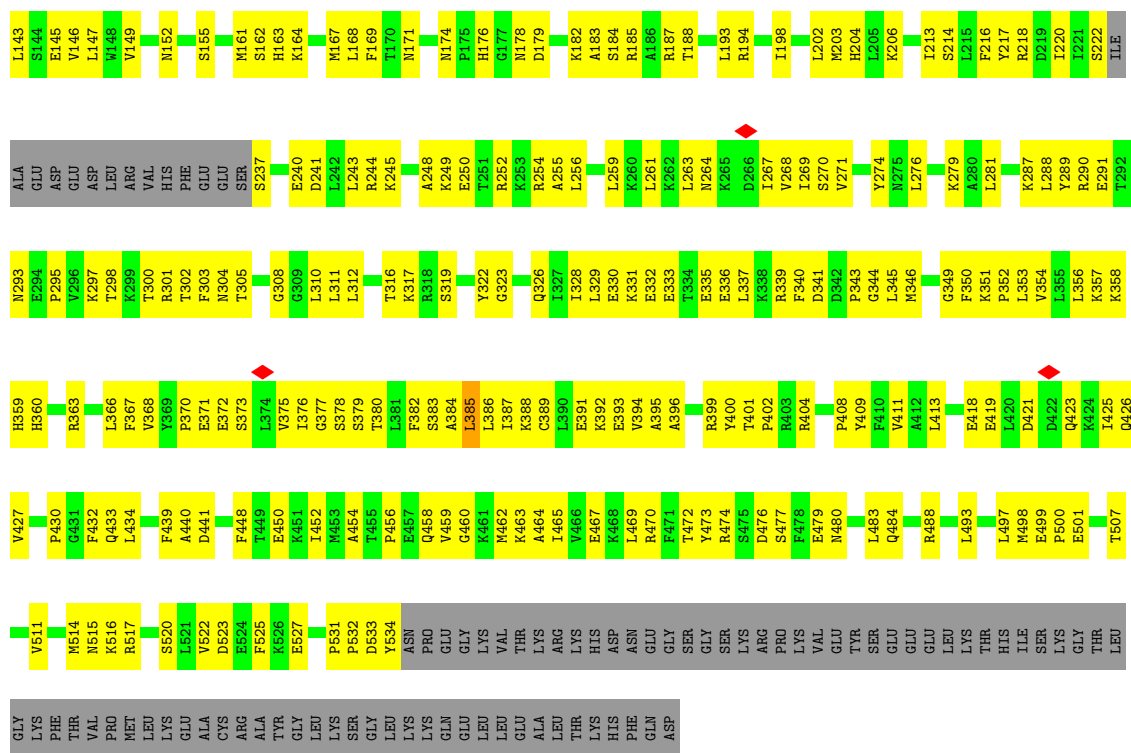
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L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	
L2901	P2902	ALA	GLU	LEU	PRO	ALA	LYS	ARG	VAL	GLY	ALA	LYS	VAL	ARG	THR	GLY	ALA	ARG	THR	PRO	MET	ARG	ASP	GLN	GLU	LYS	THR	PHE	THR	GLY	ALA	ARG	GLU	GLN	LYS	ILE	LYS	SER	GLU	LYS	LEU	LYS	MET	LYS	GLN	ASP	A2767	ASP	



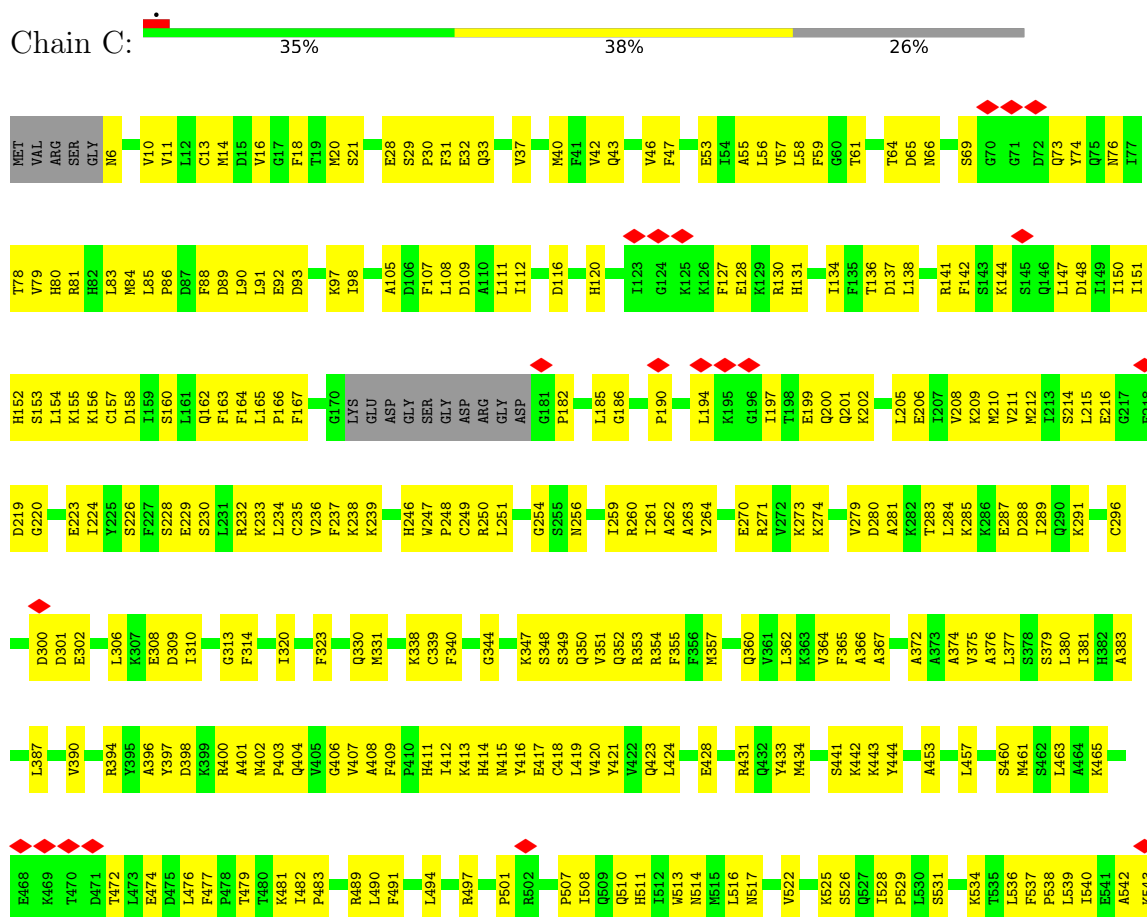
● Molecule 2: X-ray repair cross-complementing protein 6

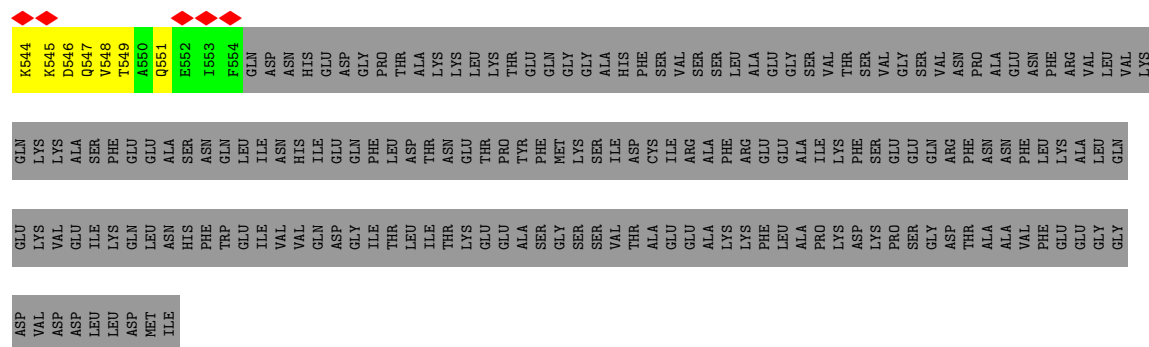
Chain B: 35% 45% 20%



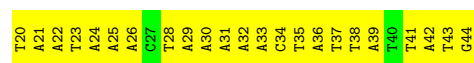


• Molecule 3: X-ray repair cross-complementing protein 5





- Molecule 4: DNA



- Molecule 5: DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59967	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.97	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.525	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.125	Depositor
Map size ($\text{\AA}$)	356.99997, 356.99997, 356.99997	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/29576	0.52	5/40030 (0.0%)
2	B	0.32	0/3984	0.50	0/5371
3	C	0.26	0/4346	0.45	0/5867
4	D	0.40	0/573	0.46	0/882
5	E	0.40	0/544	0.53	0/837
All	All	0.38	0/39023	0.51	5/52987 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2351	GLN	N-CA-C	-8.54	100.98	111.40
1	A	3671	ASN	N-CA-C	-7.94	100.61	112.04
1	A	4028	ILE	N-CA-C	-7.71	105.33	112.43
1	A	126	PRO	N-CA-CB	6.82	110.76	103.39
1	A	2330	VAL	N-CA-C	5.04	119.82	109.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29124	0	29016	1375	0
2	B	3908	0	3962	265	0
3	C	4260	0	4262	268	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	510	0	286	24	0
5	E	487	0	279	23	0
All	All	38289	0	37805	1887	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1887) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3472:ILE:HG21	1:A:3483:MET:CE	1.54	1.36
1:A:2330:VAL:CB	1:A:2336:ILE:HG22	1.55	1.35
1:A:2330:VAL:HG23	1:A:2335:ASN:O	1.31	1.25
2:B:370:PRO:HB3	2:B:382:PHE:CD2	1.76	1.21
1:A:2330:VAL:HB	1:A:2336:ILE:CG2	1.72	1.20
1:A:3472:ILE:HG21	1:A:3483:MET:HE3	1.29	1.07
1:A:3472:ILE:CG2	1:A:3483:MET:CE	2.33	1.06
1:A:1376:LEU:HD13	1:A:1403:MET:HE1	1.04	1.03
1:A:1376:LEU:HD13	1:A:1403:MET:CE	1.88	1.01
1:A:2124:SER:HA	1:A:2127:LYS:HB2	1.44	0.98
1:A:1352:SER:CB	1:A:1353:PRO:CD	2.43	0.96
1:A:442:GLN:NE2	1:A:457:CYS:SG	2.41	0.94
1:A:1376:LEU:CD1	1:A:1403:MET:HE1	1.97	0.93
1:A:263:LYS:HB3	1:A:265:TYR:CE1	2.06	0.91
1:A:3015:SER:OG	1:A:3044:MET:SD	2.29	0.90
1:A:1356:TRP:HB3	1:A:1359:LEU:HD21	1.53	0.90
1:A:2138:VAL:HB	1:A:2139:PRO:CD	2.02	0.90
1:A:1356:TRP:HB3	1:A:1359:LEU:CD2	2.01	0.90
2:B:370:PRO:CB	2:B:382:PHE:CD2	2.56	0.89
1:A:1482:GLU:O	1:A:1486:LEU:HB2	1.71	0.88
1:A:3472:ILE:CG2	1:A:3483:MET:HE2	2.02	0.87
1:A:384:MET:HA	1:A:387:GLU:OE1	1.74	0.86
2:B:352:PRO:HA	2:B:394:VAL:HA	1.58	0.86
1:A:1352:SER:CB	1:A:1353:PRO:HD2	2.06	0.84
1:A:2330:VAL:CB	1:A:2336:ILE:CG2	2.42	0.84
2:B:271:VAL:HG12	2:B:382:PHE:CZ	2.13	0.84
1:A:3502:MET:HB3	1:A:3514:VAL:HG21	1.59	0.84
1:A:263:LYS:HE3	1:A:265:TYR:HE1	1.43	0.84
3:C:247:TRP:HB3	3:C:263:ALA:HB3	1.60	0.83
1:A:3417:ALA:HB1	1:A:3450:MET:HE2	1.59	0.83
1:A:3549:HIS:O	1:A:3552:LYS:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:HB	1:A:268:PRO:HD3	1.60	0.83
1:A:2330:VAL:CG2	1:A:2336:ILE:HG22	2.08	0.82
1:A:2894:GLU:HG3	1:A:3973:PRO:HG2	1.61	0.82
1:A:2368:THR:HG21	1:A:2400:VAL:HG23	1.61	0.82
1:A:1686:LEU:HA	1:A:1689:LYS:HD2	1.61	0.81
1:A:3592:VAL:HG23	1:A:3609:MET:HE2	1.63	0.81
2:B:346:MET:HB3	2:B:399:ARG:HB3	1.60	0.81
2:B:358:LYS:HB2	3:C:353:ARG:HH22	1.43	0.81
1:A:1393:ALA:O	1:A:1396:PRO:HD2	1.80	0.81
1:A:3636:PHE:HZ	1:A:3669:LYS:HD2	1.47	0.80
1:A:1389:VAL:HB	1:A:1391:VAL:HG12	1.63	0.79
2:B:458:GLN:HE22	2:B:527:GLU:HB2	1.47	0.79
1:A:2138:VAL:HB	1:A:2139:PRO:HD2	1.64	0.79
1:A:3256:MET:HE1	1:A:3287:ARG:HH21	1.47	0.78
3:C:306:LEU:HG	3:C:308:GLU:H	1.47	0.77
1:A:1013:ILE:HG23	1:A:1014:LEU:HD12	1.64	0.77
3:C:235:CYS:SG	3:C:239:LYS:NZ	2.57	0.77
1:A:3281:CYS:O	1:A:3285:HIS:HB2	1.83	0.77
3:C:136:THR:HG22	3:C:138:LEU:H	1.50	0.77
1:A:1804:MET:HA	1:A:1807:LYS:HB2	1.68	0.76
2:B:302:THR:HA	3:C:291:LYS:HA	1.67	0.76
1:A:3243:ILE:HD11	1:A:3258:LEU:HD22	1.66	0.76
1:A:1321:ARG:NH1	1:A:1321:ARG:O	2.18	0.76
1:A:3710:LYS:NZ	1:A:3711:PRO:O	2.18	0.76
1:A:2330:VAL:HB	1:A:2336:ILE:HG22	0.79	0.75
1:A:3288:SER:OG	1:A:3289:ARG:NH1	2.20	0.75
3:C:58:LEU:HD13	3:C:80:HIS:HB2	1.69	0.75
2:B:349:GLY:HA2	3:C:461:MET:HE1	1.68	0.75
1:A:263:LYS:HE3	1:A:265:TYR:CE1	2.22	0.75
1:A:3472:ILE:HG21	1:A:3483:MET:HE1	1.66	0.75
1:A:2254:ARG:NH2	1:A:2292:CYS:SG	2.59	0.74
1:A:211:ALA:HB3	3:C:548:VAL:HA	1.67	0.74
1:A:1338:VAL:HA	1:A:1341:ILE:HD12	1.68	0.74
2:B:125:GLN:OE1	2:B:129:LYS:NZ	2.21	0.74
2:B:458:GLN:HB3	2:B:462:MET:HE1	1.69	0.74
2:B:106:GLN:NE2	2:B:118:GLU:OE1	2.21	0.74
2:B:240:GLU:HA	2:B:243:LEU:HD12	1.68	0.74
3:C:280:ASP:HB2	3:C:289:ILE:HD11	1.69	0.73
1:A:4027:TRP:HA	1:A:4029:GLN:HE22	1.51	0.73
1:A:2365:ASN:ND2	1:A:2399:GLU:OE2	2.21	0.73
1:A:2426:HIS:O	1:A:2432:GLN:NE2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3367:SER:HB2	1:A:3373:VAL:HG22	1.69	0.73
2:B:35:ARG:NH1	2:B:80:ARG:O	2.22	0.73
2:B:419:GLU:O	2:B:426:GLN:NE2	2.21	0.73
1:A:2216:LEU:HD22	1:A:2249:LEU:HD12	1.69	0.73
2:B:384:ALA:C	2:B:386:LEU:H	1.96	0.73
1:A:2330:VAL:CG2	1:A:2336:ILE:CG2	2.66	0.73
1:A:3363:SER:O	1:A:3380:ARG:NH1	2.22	0.73
2:B:511:VAL:HA	2:B:514:MET:HB2	1.70	0.73
1:A:167:PRO:HB2	1:A:171:LEU:HD22	1.71	0.72
1:A:656:GLN:OE1	1:A:659:ARG:NH2	2.22	0.72
1:A:3518:VAL:HA	1:A:3521:ILE:HG22	1.71	0.72
4:D:29:DA:H2''	4:D:30:DA:H5'	1.72	0.72
1:A:1836:LEU:HB3	1:A:1880:MET:HE1	1.70	0.72
1:A:3875:GLU:O	1:A:3965:ARG:NH1	2.22	0.72
1:A:2244:CYS:HG	1:A:2245:TRP:CD1	2.07	0.72
2:B:131:PHE:HA	2:B:134:MET:HG3	1.69	0.71
2:B:385:LEU:HA	2:B:392:LYS:HG2	1.72	0.71
1:A:1855:PHE:HA	1:A:1863:PHE:HZ	1.54	0.71
2:B:178:ASN:HD22	2:B:182:LYS:HB3	1.55	0.71
1:A:737:PRO:HD2	1:A:740:ILE:HD12	1.73	0.71
1:A:2330:VAL:CG2	1:A:2335:ASN:O	2.26	0.71
2:B:357:LYS:HB2	2:B:360:HIS:HD2	1.54	0.71
1:A:1807:LYS:HG3	1:A:1809:ASP:H	1.55	0.71
1:A:3292:GLY:O	1:A:3296:GLN:NE2	2.23	0.71
2:B:330:GLU:HG3	2:B:332:GLU:H	1.56	0.71
2:B:289:TYR:HD2	2:B:291:GLU:H	1.38	0.71
3:C:413:LYS:N	3:C:417:GLU:OE1	2.23	0.71
1:A:1212:LEU:HB2	1:A:1216:GLY:HA3	1.73	0.71
1:A:3011:LEU:HD23	1:A:3047:SER:HB3	1.72	0.71
2:B:174:ASN:OD1	2:B:176:HIS:NE2	2.24	0.71
2:B:498:MET:HG2	2:B:499:GLU:H	1.55	0.71
2:B:174:ASN:HD22	2:B:216:PHE:HB2	1.55	0.70
2:B:389:CYS:HA	2:B:392:LYS:HB2	1.73	0.70
2:B:533:ASP:OD1	3:C:260:ARG:NH2	2.24	0.70
1:A:1356:TRP:HA	1:A:1356:TRP:CE3	2.24	0.70
1:A:3529:ILE:HG22	1:A:3533:PHE:HB2	1.73	0.70
2:B:145:GLU:OE2	2:B:185:ARG:NH2	2.24	0.70
3:C:162:GLN:NE2	3:C:163:PHE:O	2.24	0.70
1:A:1356:TRP:O	1:A:1359:LEU:HD23	1.91	0.70
2:B:41:LEU:HB3	2:B:168:LEU:HD12	1.72	0.70
2:B:261:LEU:HB3	2:B:269:ILE:HG23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3771:MET:HE1	1:A:3998:LEU:HD22	1.73	0.70
3:C:11:VAL:HG12	3:C:55:ALA:HB3	1.73	0.70
1:A:2101:VAL:HA	1:A:2104:MET:HE3	1.73	0.70
1:A:2493:ASN:O	1:A:2497:GLU:N	2.24	0.70
1:A:3672:LYS:C	1:A:3674:SER:H	1.99	0.70
1:A:3232:ARG:NH2	1:A:3268:THR:OG1	2.25	0.70
1:A:3170:ASP:N	1:A:3174:ASP:OD2	2.25	0.69
1:A:267:VAL:HB	1:A:268:PRO:CD	2.21	0.69
1:A:353:ASP:HB2	1:A:359:LEU:HD23	1.74	0.69
1:A:2268:LYS:NZ	1:A:2311:ARG:O	2.25	0.69
1:A:1298:LEU:HD13	1:A:1366:THR:HB	1.73	0.69
1:A:2405:VAL:HA	1:A:2408:MET:HE1	1.73	0.69
1:A:2424:MET:O	1:A:2432:GLN:NE2	2.26	0.69
2:B:523:ASP:OD1	3:C:256:ASN:ND2	2.26	0.69
1:A:1356:TRP:HA	1:A:1356:TRP:HE3	1.55	0.69
1:A:3496:ILE:HA	1:A:3499:ILE:HD11	1.74	0.69
1:A:721:TYR:HB2	1:A:726:LEU:HD13	1.74	0.69
1:A:1921:ASP:OD1	1:A:1922:ALA:N	2.25	0.69
3:C:165:LEU:HD12	3:C:166:PRO:HD2	1.74	0.69
3:C:76:ASN:HB2	3:C:105:ALA:HB2	1.75	0.69
1:A:803:SER:O	1:A:852:ARG:NH2	2.26	0.69
1:A:1818:SER:OG	1:A:1822:ARG:NH1	2.26	0.68
1:A:3698:GLU:HB2	1:A:3718:ARG:HD2	1.75	0.68
1:A:232:CYS:O	1:A:278:HIS:NE2	2.27	0.68
1:A:3352:GLU:HG2	1:A:3354:ASP:H	1.58	0.68
2:B:396:ALA:HB3	2:B:413:LEU:HB3	1.73	0.68
3:C:407:VAL:HB	3:C:424:LEU:HD11	1.73	0.68
2:B:179:ASP:OD1	2:B:182:LYS:N	2.26	0.68
3:C:413:LYS:HD2	3:C:415:ASN:HB2	1.74	0.68
1:A:80:GLU:HA	1:A:83:GLU:HG2	1.76	0.68
2:B:50:GLU:OE2	2:B:53:SER:N	2.26	0.68
3:C:134:ILE:HB	3:C:163:PHE:HA	1.76	0.68
1:A:1226:GLY:HA2	1:A:1234:GLY:HA3	1.75	0.68
1:A:2295:GLN:OE1	1:A:2298:GLU:N	2.25	0.68
2:B:462:MET:HG3	2:B:465:ILE:HD12	1.76	0.68
5:E:23:DT:H2''	5:E:24:DT:H5''	1.73	0.68
2:B:370:PRO:HB3	2:B:382:PHE:CG	2.29	0.68
1:A:999:LYS:NZ	1:A:2581:LEU:O	2.25	0.67
2:B:370:PRO:HB3	2:B:382:PHE:CE2	2.28	0.67
2:B:379:SER:HA	2:B:382:PHE:HB2	1.74	0.67
1:A:1945:TYR:HE2	1:A:2097:LEU:HD21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3450:MET:SD	1:A:3468:LEU:HD11	2.34	0.67
2:B:264:ASN:HD21	2:B:267:ILE:HG23	1.59	0.67
1:A:3559:LYS:O	1:A:3564:GLN:NE2	2.25	0.67
1:A:584:GLU:O	1:A:613:HIS:N	2.25	0.67
1:A:1458:LEU:O	1:A:1462:GLY:N	2.26	0.67
1:A:3622:ALA:HB3	1:A:3625:LEU:HB3	1.75	0.67
1:A:3669:LYS:C	1:A:3671:ASN:H	2.01	0.67
3:C:37:VAL:HA	3:C:40:MET:SD	2.34	0.67
1:A:1725:GLN:OE1	1:A:1727:ARG:N	2.28	0.67
2:B:357:LYS:HB2	2:B:360:HIS:CD2	2.30	0.67
2:B:366:LEU:HB2	2:B:434:LEU:HB2	1.76	0.67
4:D:28:DT:H2'	4:D:29:DA:C8	2.30	0.67
1:A:538:ASP:OD2	1:A:539:GLN:NE2	2.29	0.66
1:A:977:ASP:OD1	1:A:978:GLN:N	2.27	0.66
2:B:317:LYS:O	3:C:279:VAL:N	2.26	0.66
1:A:2330:VAL:HG23	1:A:2335:ASN:C	2.18	0.66
1:A:2540:LEU:HD11	1:A:2832:ILE:HG23	1.76	0.66
1:A:3390:GLN:NE2	1:A:3393:GLU:OE2	2.27	0.66
2:B:511:VAL:HG21	3:C:254:GLY:HA2	1.76	0.66
1:A:2986:PRO:O	1:A:2991:LYS:NZ	2.28	0.66
1:A:3179:TRP:HB3	1:A:3242:MET:HE3	1.77	0.66
2:B:351:LYS:O	2:B:395:ALA:N	2.25	0.66
3:C:152:HIS:HA	3:C:155:LYS:HG2	1.76	0.66
2:B:384:ALA:O	2:B:386:LEU:N	2.28	0.66
1:A:356:ASN:O	1:A:406:ARG:NH1	2.29	0.66
1:A:2330:VAL:O	1:A:2336:ILE:HA	1.95	0.66
1:A:3446:VAL:HG22	1:A:3450:MET:HE3	1.77	0.66
1:A:60:SER:HA	1:A:63:PHE:HB3	1.76	0.66
1:A:2122:LEU:H	1:A:2160:TYR:HE2	1.44	0.66
3:C:89:ASP:OD1	3:C:90:LEU:N	2.27	0.66
1:A:3297:VAL:HG23	1:A:3298:LEU:HD12	1.77	0.66
1:A:3867:THR:OG1	1:A:4119:ARG:NH2	2.29	0.66
3:C:151:ILE:HD12	3:C:154:LEU:HD11	1.78	0.66
3:C:235:CYS:HA	3:C:238:LYS:HG2	1.77	0.66
1:A:1414:ILE:O	1:A:1418:HIS:ND1	2.20	0.65
3:C:330:GLN:NE2	3:C:331:MET:SD	2.69	0.65
1:A:1102:GLU:OE1	1:A:1152:ARG:NH1	2.29	0.65
1:A:1840:PHE:HB2	1:A:1880:MET:HE2	1.79	0.65
1:A:2327:LEU:O	1:A:2371:PHE:CD1	2.49	0.65
1:A:2967:GLU:O	1:A:2970:LYS:HB3	1.95	0.65
1:A:1623:LEU:HA	1:A:1626:TRP:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1910:GLU:O	1:A:1913:LYS:HG2	1.96	0.65
3:C:364:VAL:HB	3:C:419:LEU:HB2	1.78	0.65
1:A:194:GLU:OE1	1:A:198:ARG:NH1	2.30	0.65
1:A:1710:LEU:HA	1:A:1713:VAL:HG22	1.76	0.65
2:B:276:LEU:HD23	2:B:367:PHE:HB2	1.79	0.65
3:C:130:ARG:NH2	3:C:157:CYS:O	2.29	0.65
1:A:1413:ASP:OD1	1:A:1414:ILE:N	2.30	0.65
1:A:263:LYS:HB3	1:A:265:TYR:HE1	1.61	0.64
2:B:305:THR:N	3:C:288:ASP:OD1	2.29	0.64
2:B:323:GLY:O	2:B:326:GLN:NE2	2.30	0.64
1:A:1406:LEU:HD13	1:A:1415:LEU:HD21	1.79	0.64
1:A:3612:ARG:HD2	1:A:3799:ARG:HH22	1.61	0.64
1:A:3958:LEU:O	1:A:4110:GLN:NE2	2.30	0.64
1:A:4040:PRO:HA	1:A:4043:LYS:HB2	1.79	0.64
3:C:216:GLU:OE1	3:C:220:GLY:N	2.30	0.64
1:A:3255:ALA:HB1	1:A:3283:LEU:HD11	1.78	0.64
1:A:3591:ASP:HB2	1:A:3609:MET:HE1	1.80	0.64
1:A:1751:GLU:OE2	1:A:1784:ARG:NE	2.31	0.64
3:C:6:ASN:N	3:C:128:GLU:OE1	2.30	0.64
3:C:347:LYS:HG3	3:C:349:SER:H	1.62	0.64
4:D:41:DT:H3	5:E:17:DT:H3	1.46	0.64
1:A:12:LEU:HD13	1:A:15:LEU:HD12	1.80	0.64
1:A:799:TYR:O	1:A:852:ARG:NH1	2.31	0.64
1:A:71:LYS:O	1:A:82:ARG:NH2	2.31	0.64
1:A:2538:ARG:NH1	1:A:2561:PHE:O	2.31	0.63
1:A:3673:ASP:O	1:A:3675:LYS:HG2	1.98	0.63
1:A:4027:TRP:HA	1:A:4029:GLN:NE2	2.13	0.63
3:C:489:ARG:NH1	3:C:507:PRO:O	2.31	0.63
1:A:638:GLN:OE1	1:A:640:GLU:N	2.28	0.63
1:A:1933:LEU:HD21	1:A:1937:ARG:HH12	1.63	0.63
3:C:250:ARG:HG2	3:C:260:ARG:HG3	1.80	0.63
1:A:1583:MET:HE1	1:A:1629:CYS:HB2	1.79	0.63
1:A:1978:PHE:HD2	1:A:1979:GLU:HG3	1.63	0.63
1:A:3085:GLU:OE1	1:A:3085:GLU:N	2.29	0.63
2:B:388:LYS:O	2:B:392:LYS:HD3	1.98	0.63
1:A:333:MET:SD	1:A:334:HIS:ND1	2.71	0.63
1:A:2952:ILE:HD13	1:A:2975:ALA:HB2	1.79	0.63
3:C:263:ALA:HB1	3:C:362:LEU:HD21	1.79	0.63
1:A:2330:VAL:HG21	1:A:2336:ILE:HG23	1.80	0.63
1:A:3101:TYR:O	1:A:3105:ASN:ND2	2.32	0.63
1:A:1471:GLN:HB3	1:A:1477:HIS:HD2	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3542:PHE:HZ	1:A:3555:VAL:HG21	1.62	0.63
1:A:3778:ASP:OD1	1:A:3779:SER:N	2.31	0.63
2:B:142:SER:HB2	2:B:145:GLU:HG2	1.80	0.63
1:A:475:LEU:HD22	1:A:476:ARG:HD2	1.80	0.63
1:A:1976:LEU:HD11	1:A:2145:PHE:CD2	2.34	0.63
1:A:2411:LEU:H	1:A:2411:LEU:HD23	1.64	0.63
1:A:3048:LYS:HB2	1:A:3061:LEU:HD13	1.81	0.63
3:C:206:GLU:HG2	3:C:209:LYS:HZ3	1.63	0.63
1:A:3306:LEU:O	1:A:3310:ASN:N	2.32	0.62
3:C:182:PRO:HB2	3:C:190:PRO:HG3	1.80	0.62
1:A:1873:TYR:HA	1:A:1876:ILE:HG12	1.81	0.62
1:A:1690:GLY:O	1:A:1745:LYS:NZ	2.26	0.62
2:B:317:LYS:HB3	2:B:328:ILE:HD11	1.81	0.62
1:A:1093:GLU:HG2	1:A:1094:SER:N	2.15	0.62
3:C:116:ASP:O	3:C:120:HIS:ND1	2.31	0.62
1:A:392:CYS:HG	1:A:413:PHE:HE1	1.48	0.62
1:A:1643:MET:HG3	1:A:1688:LEU:HD13	1.81	0.62
1:A:1892:LYS:HD2	1:A:1907:GLU:HG2	1.81	0.62
2:B:344:GLY:N	2:B:401:THR:OG1	2.33	0.62
3:C:548:VAL:O	3:C:551:GLN:NE2	2.33	0.62
1:A:1442:GLN:HA	1:A:1445:ARG:HD3	1.81	0.62
1:A:1711:ARG:HH12	1:A:1757:MET:HG3	1.64	0.62
1:A:3176:MET:HE2	1:A:3246:ALA:HB2	1.81	0.62
1:A:3295:GLU:OE1	1:A:3295:GLU:N	2.26	0.62
1:A:4049:ARG:HH21	1:A:4059:ILE:HD13	1.65	0.62
3:C:81:ARG:HH21	3:C:84:MET:HG2	1.64	0.62
1:A:332:GLU:O	1:A:335:LYS:NZ	2.30	0.62
1:A:1878:ASP:HB3	1:A:1947:CYS:HA	1.81	0.62
3:C:141:ARG:NH2	3:C:200:GLN:OE1	2.32	0.62
3:C:463:LEU:HD12	3:C:477:PHE:HB2	1.81	0.62
1:A:239:GLU:H	1:A:243:GLN:HE22	1.46	0.62
1:A:3483:MET:O	1:A:3487:ILE:HG12	2.00	0.62
1:A:3508:LYS:HD3	1:A:3509:ASP:N	2.14	0.62
3:C:56:LEU:O	3:C:80:HIS:N	2.32	0.62
2:B:375:VAL:HG23	3:C:540:ILE:H	1.65	0.62
1:A:2124:SER:O	1:A:2128:PHE:N	2.31	0.62
1:A:3652:LEU:HG	1:A:3653:ARG:HD2	1.81	0.62
1:A:3981:TYR:HB2	1:A:4108:MET:HE1	1.80	0.61
1:A:147:PHE:HE2	1:A:148:LYS:HE3	1.65	0.61
1:A:3550:LYS:O	1:A:3553:GLU:HG3	2.00	0.61
1:A:3636:PHE:CZ	1:A:3669:LYS:HD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3653:ARG:HA	1:A:3659:PHE:CG	2.34	0.61
1:A:4127:TRP:CD1	1:A:4128:MET:H	2.18	0.61
1:A:3820:MET:HB3	1:A:3882:LEU:HD11	1.83	0.61
2:B:399:ARG:NH1	3:C:516:LEU:O	2.30	0.61
1:A:3643:HIS:O	1:A:3653:ARG:NH2	2.33	0.61
1:A:1250:LEU:HD22	1:A:1319:GLY:HA2	1.81	0.61
1:A:1583:MET:HG3	1:A:1628:LYS:HB2	1.83	0.61
1:A:2825:THR:N	1:A:2828:GLU:OE2	2.32	0.61
1:A:449:TYR:HB3	1:A:453:MET:SD	2.40	0.61
1:A:1565:GLU:OE1	1:A:1565:GLU:N	2.29	0.61
1:A:2205:VAL:HG12	1:A:2208:ASP:H	1.66	0.61
2:B:337:LEU:HD11	3:C:490:LEU:HA	1.82	0.61
1:A:718:MET:HE2	1:A:726:LEU:HD11	1.82	0.61
1:A:1312:CYS:SG	1:A:1313:PHE:N	2.71	0.61
1:A:3344:GLU:HG3	1:A:3347:CYS:H	1.66	0.61
2:B:271:VAL:CG1	2:B:382:PHE:CZ	2.83	0.61
3:C:542:ALA:O	3:C:545:LYS:NZ	2.34	0.61
1:A:188:GLU:O	1:A:192:ASN:ND2	2.34	0.61
1:A:305:ASN:O	1:A:309:LYS:NZ	2.32	0.61
2:B:358:LYS:HA	3:C:353:ARG:HH12	1.65	0.61
3:C:406:GLY:HA2	3:C:424:LEU:HG	1.83	0.61
2:B:263:LEU:HD11	2:B:267:ILE:HD11	1.82	0.61
3:C:442:LYS:HB2	3:C:443:LYS:HZ2	1.65	0.61
1:A:2146:LEU:HD13	1:A:2149:LEU:HD12	1.83	0.61
1:A:2253:TYR:HA	1:A:2256:ILE:HD12	1.81	0.61
2:B:288:LEU:HD23	2:B:293:ASN:HA	1.81	0.60
2:B:319:SER:HB2	3:C:279:VAL:HG21	1.82	0.60
2:B:322:TYR:HE2	3:C:47:PHE:HA	1.66	0.60
2:B:330:GLU:N	2:B:333:GLU:OE2	2.27	0.60
2:B:522:VAL:HA	2:B:525:PHE:HB2	1.82	0.60
1:A:70:ARG:HH12	1:A:72:SER:HA	1.66	0.60
1:A:1142:HIS:O	1:A:1146:ASN:N	2.28	0.60
1:A:2304:VAL:O	1:A:2307:MET:HG3	2.00	0.60
1:A:257:ARG:HH11	1:A:261:ASP:HB3	1.65	0.60
1:A:363:ILE:HD12	1:A:413:PHE:HA	1.82	0.60
1:A:469:ALA:HA	1:A:475:LEU:HG	1.82	0.60
1:A:1945:TYR:CE2	1:A:1949:ILE:HD11	2.37	0.60
1:A:2429:ASP:OD1	1:A:2430:GLU:N	2.34	0.60
3:C:108:LEU:HD23	3:C:111:LEU:HD12	1.82	0.60
1:A:1639:LEU:HD23	1:A:1643:MET:HE1	1.83	0.60
3:C:248:PRO:HA	3:C:262:ALA:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HG3	1:A:185:HIS:H	1.64	0.60
1:A:352:VAL:HG11	1:A:1735:ARG:HB2	1.82	0.60
1:A:395:MET:HE2	1:A:406:ARG:HD2	1.84	0.60
1:A:1049:GLN:O	1:A:1055:ASN:ND2	2.27	0.60
2:B:384:ALA:C	2:B:386:LEU:N	2.59	0.60
1:A:3586:LYS:HE3	1:A:3667:LEU:HD13	1.82	0.60
2:B:433:GLN:HE22	3:C:353:ARG:HB3	1.66	0.60
1:A:1619:ALA:HA	1:A:1652:ILE:HD11	1.84	0.60
1:A:1588:ASP:OD1	1:A:1589:ASN:N	2.34	0.60
1:A:1892:LYS:O	1:A:1908:GLY:N	2.28	0.60
1:A:3108:GLN:HA	1:A:3111:MET:SD	2.42	0.60
1:A:4017:GLU:O	1:A:4021:LEU:HG	2.01	0.60
2:B:263:LEU:HD23	2:B:263:LEU:H	1.66	0.60
1:A:1724:MET:HA	1:A:1768:ARG:HH11	1.67	0.60
1:A:2821:ASP:HB2	1:A:2822:LYS:HZ2	1.66	0.60
1:A:3646:LYS:NZ	1:A:3653:ARG:HH12	1.99	0.60
3:C:57:VAL:HA	3:C:79:VAL:HA	1.84	0.60
1:A:2122:LEU:HD11	1:A:2163:HIS:CD2	2.37	0.60
1:A:3645:GLY:H	1:A:3650:LYS:HZ1	1.49	0.60
2:B:271:VAL:CG1	2:B:382:PHE:HZ	2.14	0.60
5:E:18:DA:H2"	5:E:19:DA:C8	2.36	0.60
1:A:741:ILE:HG23	1:A:748:TYR:HD2	1.66	0.59
1:A:1782:PHE:HA	1:A:1785:ILE:HG22	1.84	0.59
1:A:2227:LYS:HZ2	1:A:2229:ALA:H	1.48	0.59
1:A:3465:PHE:HA	1:A:3468:LEU:HD13	1.84	0.59
2:B:467:GLU:HA	2:B:470:ARG:HH12	1.66	0.59
1:A:61:ARG:NH1	1:A:106:GLU:OE1	2.35	0.59
1:A:234:PHE:O	1:A:281:GLN:NE2	2.34	0.59
1:A:586:GLN:N	1:A:611:ASN:O	2.36	0.59
1:A:1093:GLU:HA	1:A:1096:VAL:HG12	1.84	0.59
1:A:1374:GLN:NE2	1:A:1378:GLU:OE2	2.35	0.59
1:A:1723:PRO:HG2	1:A:1729:PHE:CZ	2.37	0.59
1:A:1769:GLU:O	1:A:1822:ARG:NH2	2.35	0.59
1:A:1955:VAL:HG22	1:A:1956:PHE:H	1.66	0.59
1:A:2330:VAL:HG21	1:A:2336:ILE:CG2	2.32	0.59
1:A:3361:GLU:OE1	1:A:3361:GLU:N	2.30	0.59
1:A:1493:PRO:HB3	1:A:1500:LEU:HA	1.83	0.59
1:A:1935:GLU:HG2	1:A:1936:ARG:HD2	1.83	0.59
1:A:2227:LYS:NZ	1:A:2229:ALA:H	2.00	0.59
1:A:3040:TYR:HB3	1:A:3044:MET:HE1	1.84	0.59
1:A:1857:LYS:HZ1	1:A:1863:PHE:HD1	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3553:GLU:O	1:A:3557:ARG:N	2.33	0.59
1:A:1863:PHE:HA	1:A:1866:GLN:OE1	2.02	0.59
1:A:3064:PHE:O	1:A:3068:ALA:HB2	2.01	0.59
1:A:3828:TYR:OH	1:A:4127:TRP:NE1	2.34	0.59
1:A:71:LYS:HD2	1:A:73:LEU:HD11	1.85	0.59
1:A:475:LEU:HD13	1:A:476:ARG:NH1	2.18	0.59
2:B:94:LYS:HE2	2:B:103:TYR:CE1	2.38	0.59
1:A:1727:ARG:NH1	1:A:1772:HIS:O	2.36	0.59
1:A:3172:LYS:HB3	1:A:3248:LYS:HD2	1.84	0.59
1:A:3700:GLU:HG3	1:A:3718:ARG:HD3	1.83	0.59
3:C:545:LYS:HB3	3:C:547:GLN:HE22	1.68	0.59
1:A:67:VAL:O	1:A:70:ARG:NH1	2.36	0.59
1:A:1471:GLN:HB3	1:A:1477:HIS:CD2	2.37	0.59
1:A:1922:ALA:O	1:A:1941:HIS:NE2	2.35	0.59
5:E:30:DT:H2'	5:E:31:DT:C6	2.38	0.59
1:A:1775:GLU:OE1	1:A:1775:GLU:N	2.32	0.59
3:C:18:PHE:O	3:C:21:SER:OG	2.20	0.59
1:A:165:LYS:HE2	1:A:171:LEU:HD21	1.85	0.58
1:A:921:ALA:HB3	1:A:927:LYS:HB2	1.84	0.58
1:A:2555:LEU:HD11	1:A:2854:PHE:HA	1.84	0.58
1:A:3059:GLN:O	1:A:3063:THR:OG1	2.20	0.58
1:A:3511:ALA:O	1:A:3515:GLN:N	2.28	0.58
3:C:53:GLU:OE2	3:C:84:MET:N	2.37	0.58
1:A:877:ASP:HA	1:A:880:MET:HG3	1.85	0.58
1:A:1818:SER:HA	1:A:1821:ASP:HB3	1.85	0.58
1:A:1844:VAL:O	1:A:1848:ILE:HG12	2.03	0.58
1:A:2146:LEU:HA	1:A:2149:LEU:HD12	1.84	0.58
1:A:3022:GLU:OE2	1:A:3023:ASN:ND2	2.36	0.58
1:A:3531:TYR:HB2	1:A:3532:PRO:HD3	1.85	0.58
1:A:681:LYS:HB3	1:A:684:GLU:HG3	1.85	0.58
1:A:847:SER:N	1:A:850:GLU:OE2	2.33	0.58
1:A:1799:GLU:HG3	1:A:1803:GLU:OE2	2.03	0.58
2:B:217:TYR:HA	2:B:220:ILE:HD13	1.84	0.58
2:B:377:GLY:HA2	3:C:444:TYR:HE2	1.67	0.58
3:C:543:LYS:HG3	3:C:544:LYS:H	1.68	0.58
1:A:3265:GLU:OE1	1:A:3265:GLU:N	2.36	0.58
1:A:131:LEU:HA	1:A:134:LEU:HD12	1.84	0.58
1:A:3018:SER:OG	1:A:3031:TRP:NE1	2.36	0.58
1:A:2891:ARG:HG3	1:A:3894:PRO:HB3	1.84	0.58
2:B:40:PHE:HD2	2:B:85:VAL:HG22	1.68	0.58
1:A:189:MET:O	1:A:193:ALA:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASN:HD21	1:A:556:SER:HB2	1.68	0.58
1:A:1913:LYS:O	1:A:1916:ILE:HG22	2.04	0.58
2:B:472:THR:O	3:C:350:GLN:NE2	2.36	0.58
3:C:479:THR:HA	3:C:482:ILE:HD12	1.85	0.58
1:A:333:MET:SD	1:A:334:HIS:N	2.77	0.58
1:A:356:ASN:HA	1:A:406:ARG:NH2	2.19	0.58
1:A:860:GLY:HA3	1:A:3136:THR:OG1	2.04	0.58
1:A:1373:VAL:O	1:A:1377:CYS:N	2.23	0.58
1:A:1497:ARG:NE	1:A:1497:ARG:HA	2.18	0.58
1:A:3607:GLU:HA	1:A:3610:TYR:CE2	2.39	0.58
1:A:4127:TRP:CD1	1:A:4128:MET:HG2	2.39	0.58
1:A:176:GLU:HA	1:A:227:LEU:HD13	1.85	0.58
1:A:3472:ILE:HD13	1:A:3483:MET:HE1	1.86	0.58
1:A:3588:TRP:NE1	1:A:3613:MET:HB3	2.19	0.58
1:A:3588:TRP:CD1	1:A:3609:MET:HE3	2.39	0.58
3:C:209:LYS:HE2	3:C:210:MET:HE3	1.86	0.58
1:A:231:LEU:O	1:A:233:ASN:N	2.35	0.58
1:A:1820:VAL:HA	1:A:1824:LEU:HB3	1.86	0.58
1:A:1938:ARG:HD2	1:A:1977:ILE:HB	1.86	0.58
2:B:167:MET:HE1	2:B:169:PHE:CZ	2.39	0.58
2:B:271:VAL:HG12	2:B:382:PHE:CE2	2.39	0.58
2:B:328:ILE:O	2:B:329:LEU:HD23	2.04	0.58
1:A:196:LEU:HG	1:A:200:PHE:CE2	2.39	0.57
1:A:2577:PHE:O	1:A:2784:GLN:NE2	2.37	0.57
4:D:42:DA:C6	5:E:14:DT:H1'	2.38	0.57
1:A:1218:SER:HA	1:A:1221:ILE:HD12	1.85	0.57
1:A:1765:VAL:HA	1:A:1768:ARG:HH21	1.69	0.57
1:A:3459:ASN:OD1	1:A:3460:GLU:N	2.37	0.57
2:B:263:LEU:HD21	2:B:267:ILE:HG13	1.86	0.57
3:C:404:GLN:HB3	3:C:423:GLN:HG3	1.85	0.57
1:A:278:HIS:HD2	1:A:281:GLN:HG3	1.69	0.57
1:A:1261:LEU:HD13	1:A:1337:VAL:HA	1.86	0.57
1:A:1427:SER:HA	1:A:1430:GLU:OE2	2.04	0.57
1:A:2576:MET:HE3	1:A:2785:ILE:HG13	1.85	0.57
1:A:3271:ASP:OD1	1:A:3272:TRP:N	2.37	0.57
1:A:3855:TYR:O	1:A:3858:MET:HG3	2.04	0.57
2:B:86:VAL:HG22	2:B:104:VAL:HA	1.85	0.57
1:A:175:TYR:O	1:A:178:LEU:HB2	2.03	0.57
1:A:2196:TRP:HB2	1:A:2199:LEU:HB2	1.85	0.57
1:A:3718:ARG:H	1:A:3743:HIS:CD2	2.22	0.57
2:B:290:ARG:NH1	3:C:310:ILE:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:MET:HB3	2:B:517:ARG:HH21	1.69	0.57
1:A:1576:ASP:OD1	1:A:1577:LEU:N	2.36	0.57
1:A:1915:LEU:HA	1:A:1918:LEU:HD12	1.87	0.57
1:A:3699:LEU:HB3	1:A:3719:ILE:HD12	1.87	0.57
2:B:90:THR:HG21	2:B:103:TYR:HB2	1.86	0.57
1:A:196:LEU:HG	1:A:200:PHE:HE2	1.69	0.57
1:A:1479:VAL:HG21	1:A:1521:PHE:CE1	2.39	0.57
3:C:352:GLN:HB3	3:C:354:ARG:HG2	1.86	0.57
1:A:1297:PHE:HD1	1:A:1300:SER:HB3	1.68	0.57
1:A:3693:GLU:HB2	1:A:3696:ARG:HD3	1.86	0.57
3:C:165:LEU:H	3:C:226:SER:HA	1.70	0.57
3:C:457:LEU:HD22	3:C:529:PRO:HB3	1.86	0.57
1:A:234:PHE:HB2	1:A:236:LYS:NZ	2.20	0.57
1:A:237:SER:O	1:A:243:GLN:NE2	2.38	0.57
1:A:801:LYS:HD2	1:A:3115:SER:HA	1.87	0.57
1:A:886:TRP:HA	1:A:964:ARG:NH1	2.19	0.57
1:A:2220:MET:SD	1:A:2252:PRO:HG3	2.45	0.57
1:A:2962:ARG:HG3	1:A:4101:GLU:OE2	2.04	0.57
1:A:3058:ASP:OD1	1:A:3059:GLN:N	2.38	0.57
1:A:3066:ASP:OD1	1:A:3067:LYS:N	2.37	0.57
1:A:341:PHE:HB3	1:A:369:PHE:CE2	2.39	0.57
1:A:1853:SER:HA	1:A:1855:PHE:CE2	2.39	0.57
1:A:2123:PRO:HB2	1:A:2125:TRP:CD1	2.40	0.57
1:A:781:ASP:OD1	1:A:781:ASP:N	2.38	0.57
1:A:1208:LEU:HG	1:A:1212:LEU:HD23	1.87	0.57
1:A:1335:CYS:SG	1:A:1382:ILE:HA	2.45	0.57
1:A:2386:LEU:HD23	1:A:2418:LYS:HB3	1.87	0.57
3:C:56:LEU:N	3:C:81:ARG:O	2.31	0.57
1:A:1202:ARG:HD3	1:A:1206:LEU:HD22	1.86	0.56
1:A:1352:SER:CB	1:A:1353:PRO:HD3	2.34	0.56
1:A:2866:ALA:HA	1:A:2869:LEU:HD12	1.87	0.56
3:C:406:GLY:HA3	3:C:421:TYR:HE1	1.69	0.56
1:A:1148:ALA:HB2	1:A:1164:CYS:HB3	1.87	0.56
1:A:1834:ASP:HA	1:A:1837:ARG:HG2	1.87	0.56
1:A:2411:LEU:O	1:A:2415:LEU:N	2.35	0.56
1:A:3035:PHE:HA	1:A:3038:GLU:HG2	1.86	0.56
1:A:3256:MET:CE	1:A:3287:ARG:HH21	2.15	0.56
1:A:3723:ASP:OD1	1:A:3741:ARG:NH1	2.38	0.56
2:B:297:LYS:N	3:C:296:CYS:O	2.37	0.56
1:A:290:TYR:OH	1:A:337:LYS:HA	2.05	0.56
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:LEU:HD13	1:A:1127:CYS:HB2	1.86	0.56
1:A:1804:MET:N	1:A:1804:MET:SD	2.78	0.56
1:A:3033:GLU:HB2	1:A:3034:PRO:HD3	1.85	0.56
1:A:3314:SER:O	1:A:3318:LYS:N	2.33	0.56
1:A:3350:GLU:N	1:A:3350:GLU:OE1	2.39	0.56
1:A:3665:MET:HA	1:A:3668:LEU:HG	1.86	0.56
1:A:3682:GLU:OE1	1:A:3682:GLU:N	2.38	0.56
2:B:252:ARG:HE	3:C:431:ARG:CZ	2.17	0.56
3:C:14:MET:SD	3:C:58:LEU:HG	2.45	0.56
3:C:16:VAL:HG11	3:C:61:THR:HB	1.87	0.56
1:A:2217:ASN:C	1:A:2221:LYS:HZ3	2.13	0.56
1:A:2291:GLN:HG2	1:A:2292:CYS:N	2.20	0.56
1:A:2313:LYS:HA	1:A:2316:TYR:CE2	2.40	0.56
1:A:4014:LYS:O	1:A:4017:GLU:N	2.38	0.56
2:B:426:GLN:HB3	3:C:434:MET:HE1	1.87	0.56
2:B:460:GLY:HA2	2:B:463:LYS:HD3	1.86	0.56
2:B:474:ARG:HB2	2:B:477:SER:HB3	1.86	0.56
3:C:163:PHE:CE2	3:C:165:LEU:HB2	2.40	0.56
1:A:753:GLN:NE2	1:A:791:ASP:HB3	2.21	0.56
3:C:465:LYS:HB2	3:C:476:LEU:HD21	1.87	0.56
3:C:508:ILE:HD13	3:C:513:TRP:NE1	2.20	0.56
1:A:349:ILE:HD13	1:A:366:TYR:CE2	2.41	0.56
1:A:3633:ILE:O	1:A:3637:GLY:N	2.23	0.56
2:B:61:ASP:OD1	2:B:124:GLY:N	2.29	0.56
3:C:58:LEU:N	3:C:78:THR:O	2.31	0.56
1:A:1058:SER:HA	1:A:1061:LYS:HG3	1.89	0.56
1:A:1221:ILE:HD13	1:A:1287:GLN:HB2	1.88	0.56
1:A:1565:GLU:H	1:A:1565:GLU:CD	2.11	0.56
3:C:14:MET:HE1	3:C:16:VAL:HB	1.88	0.56
1:A:187:SER:HA	1:A:190:ILE:HD12	1.87	0.55
1:A:762:TYR:HD2	1:A:765:LEU:HG	1.71	0.55
1:A:2271:SER:HA	1:A:2274:ILE:HD12	1.87	0.55
1:A:3512:VAL:HA	1:A:3515:GLN:HB3	1.87	0.55
1:A:3586:LYS:HE2	1:A:3586:LYS:HA	1.88	0.55
1:A:1762:MET:HA	1:A:1762:MET:HE3	1.87	0.55
1:A:1876:ILE:O	1:A:1880:MET:HG2	2.06	0.55
1:A:2354:ASN:OD1	1:A:2355:THR:N	2.32	0.55
1:A:3307:LEU:HB2	1:A:3310:ASN:O	2.06	0.55
1:A:100:ILE:O	1:A:104:SER:N	2.34	0.55
1:A:175:TYR:HB3	1:A:227:LEU:HD22	1.89	0.55
1:A:349:ILE:HD13	1:A:366:TYR:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PHE:CG	1:A:410:MET:HE1	2.42	0.55
1:A:2578:GLU:HA	1:A:2784:GLN:HE22	1.71	0.55
1:A:3771:MET:HE2	1:A:3771:MET:HA	1.88	0.55
3:C:69:SER:HA	3:C:74:TYR:HB2	1.87	0.55
1:A:240:GLU:H	1:A:243:GLN:NE2	2.04	0.55
1:A:1239:PRO:HG2	1:A:1243:TYR:CE2	2.41	0.55
1:A:3554:PHE:HA	1:A:3557:ARG:HB3	1.88	0.55
1:A:1743:MET:HA	1:A:1743:MET:HE3	1.88	0.55
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.07	0.55
1:A:2422:GLN:OE1	1:A:2425:ARG:NH2	2.39	0.55
1:A:2464:HIS:CE1	1:A:2466:SER:HB2	2.41	0.55
1:A:3831:ASP:O	1:A:3833:ARG:N	2.40	0.55
3:C:56:LEU:HB3	3:C:81:ARG:H	1.71	0.55
1:A:392:CYS:SG	1:A:413:PHE:HE1	2.30	0.55
1:A:1305:ASP:OD1	1:A:1305:ASP:N	2.39	0.55
1:A:2332:GLU:OE1	1:A:2335:ASN:N	2.39	0.55
1:A:2966:SER:OG	1:A:2967:GLU:N	2.37	0.55
1:A:3588:TRP:NE1	1:A:3609:MET:HE3	2.21	0.55
1:A:3757:ASP:OD2	1:A:3759:ARG:NH1	2.40	0.55
3:C:20:MET:HE2	3:C:31:PHE:CD1	2.41	0.55
1:A:78:PHE:HB2	1:A:82:ARG:CZ	2.37	0.55
1:A:200:PHE:CE1	1:A:227:LEU:HD21	2.42	0.55
2:B:498:MET:HG2	2:B:499:GLU:N	2.22	0.55
3:C:165:LEU:HG	3:C:167:PHE:H	1.70	0.55
1:A:1479:VAL:O	1:A:1482:GLU:HG3	2.07	0.55
1:A:1646:LEU:HD11	1:A:1692:ALA:HB2	1.88	0.55
1:A:3256:MET:HE1	1:A:3287:ARG:NH2	2.18	0.55
1:A:3460:GLU:OE2	1:A:3464:LYS:HE3	2.07	0.55
1:A:3598:LYS:HG3	1:A:3599:THR:HG22	1.88	0.55
1:A:3731:SER:O	1:A:3734:ARG:NH1	2.40	0.55
1:A:1772:HIS:N	1:A:1775:GLU:OE2	2.33	0.55
1:A:2185:MET:SD	1:A:2186:VAL:HG23	2.47	0.55
1:A:3417:ALA:HA	1:A:3446:VAL:HG23	1.89	0.55
1:A:3478:GLU:HA	1:A:3482:LEU:HD13	1.88	0.55
1:A:245:SER:HA	1:A:248:ILE:HG12	1.89	0.54
1:A:3581:PRO:HA	1:A:3584:LEU:HD12	1.89	0.54
1:A:347:GLY:O	1:A:350:ARG:NH2	2.41	0.54
1:A:1005:ASP:OD1	1:A:1005:ASP:N	2.38	0.54
1:A:2442:MET:HE1	1:A:2446:LEU:HD22	1.89	0.54
1:A:3232:ARG:HG2	1:A:3272:TRP:CH2	2.42	0.54
1:A:3650:LYS:HZ2	1:A:3653:ARG:NH1	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:GLU:O	2:B:333:GLU:HG2	2.07	0.54
3:C:259:ILE:HG21	3:C:377:LEU:HD11	1.88	0.54
3:C:490:LEU:O	3:C:494:LEU:HG	2.08	0.54
1:A:152:LEU:HA	1:A:155:LYS:HE2	1.89	0.54
1:A:195:ASN:OD1	1:A:196:LEU:N	2.40	0.54
1:A:1306:ILE:HG23	1:A:1307:ILE:HG23	1.88	0.54
2:B:423:GLN:HB2	2:B:425:ILE:HG12	1.89	0.54
3:C:43:GLN:HA	3:C:46:VAL:HG22	1.88	0.54
1:A:360:SER:O	1:A:364:ARG:HG2	2.07	0.54
1:A:876:SER:OG	1:A:879:MET:HB2	2.07	0.54
1:A:1804:MET:O	1:A:1811:ARG:NH2	2.40	0.54
1:A:3348:LEU:HA	1:A:3351:ILE:O	2.08	0.54
1:A:1860:GLU:OE1	1:A:1860:GLU:N	2.40	0.54
2:B:48:MET:N	2:B:48:MET:SD	2.75	0.54
4:D:36:DA:H61	5:E:21:DA:N6	2.04	0.54
1:A:975:ASP:OD1	1:A:976:VAL:N	2.39	0.54
1:A:3610:TYR:HA	1:A:3613:MET:HG3	1.89	0.54
2:B:161:MET:HG2	2:B:164:LYS:HG2	1.89	0.54
1:A:23:ASP:HB3	1:A:34:LEU:HD21	1.89	0.54
1:A:682:TYR:O	1:A:700:LYS:NZ	2.36	0.54
1:A:1684:LEU:O	1:A:1689:LYS:NZ	2.37	0.54
1:A:1839:PHE:O	1:A:1843:ILE:HG12	2.08	0.54
1:A:2312:TYR:O	1:A:2315:VAL:HG22	2.07	0.54
2:B:171:ASN:OD1	2:B:206:LYS:HB2	2.07	0.54
1:A:111:CYS:HB2	1:A:130:LEU:HD11	1.90	0.54
1:A:171:LEU:HD23	1:A:171:LEU:H	1.72	0.54
1:A:216:LYS:NZ	3:C:547:GLN:H	2.05	0.54
1:A:1592:MET:O	1:A:1596:VAL:N	2.27	0.54
1:A:2812:LEU:O	1:A:2816:ILE:HG12	2.08	0.54
1:A:3030:ILE:HA	1:A:3033:GLU:CD	2.33	0.54
1:A:4018:GLN:HA	1:A:4021:LEU:HD12	1.90	0.54
2:B:480:ASN:OD1	2:B:483:LEU:N	2.32	0.54
3:C:28:GLU:HB3	3:C:32:GLU:OE2	2.07	0.54
1:A:767:GLU:CD	1:A:771:ASN:HD21	2.14	0.54
1:A:2556:SER:O	1:A:2559:THR:OG1	2.24	0.54
3:C:134:ILE:N	3:C:162:GLN:O	2.41	0.54
3:C:460:SER:O	3:C:525:LYS:NZ	2.30	0.54
4:D:21:DA:H2"	4:D:22:DA:C8	2.42	0.54
1:A:164:LYS:O	1:A:166:ILE:HD12	2.08	0.54
1:A:1195:VAL:HG11	1:A:1204:PRO:HA	1.90	0.54
1:A:1848:ILE:O	1:A:1852:LYS:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2962:ARG:NH1	1:A:4101:GLU:OE1	2.41	0.54
3:C:270:GLU:OE2	3:C:273:LYS:NZ	2.40	0.54
3:C:381:ILE:HD12	3:C:417:GLU:HB2	1.89	0.54
1:A:112:THR:O	1:A:116:THR:N	2.41	0.53
1:A:211:ALA:HB1	1:A:215:PRO:HA	1.90	0.53
1:A:432:THR:OG1	1:A:433:PRO:HD3	2.08	0.53
1:A:663:ILE:HG22	1:A:665:GLY:H	1.72	0.53
1:A:1297:PHE:CD1	1:A:1300:SER:HB3	2.42	0.53
1:A:3700:GLU:HA	1:A:3718:ARG:HA	1.89	0.53
1:A:3949:ALA:O	1:A:3953:LEU:HD12	2.08	0.53
2:B:102:ILE:HD13	2:B:149:VAL:HG21	1.90	0.53
1:A:220:LEU:O	1:A:224:LEU:HG	2.07	0.53
1:A:3494:GLN:O	1:A:3495:PHE:HB2	2.08	0.53
1:A:754:MET:HA	1:A:754:MET:HE2	1.90	0.53
2:B:520:SER:OG	2:B:523:ASP:OD2	2.26	0.53
3:C:411:HIS:HB2	3:C:420:VAL:HG23	1.90	0.53
1:A:1414:ILE:HG13	1:A:1415:LEU:HD22	1.90	0.53
1:A:1722:PHE:HD1	1:A:1739:TYR:CE1	2.26	0.53
1:A:2227:LYS:HB3	1:A:2230:VAL:HG12	1.90	0.53
1:A:2333:ARG:C	1:A:2334:LYS:HD3	2.33	0.53
3:C:40:MET:HB2	3:C:43:GLN:HE21	1.74	0.53
1:A:1629:CYS:HG	1:A:1632:TRP:CG	2.27	0.53
1:A:1686:LEU:HD11	1:A:1721:HIS:CD2	2.43	0.53
1:A:1711:ARG:NH1	1:A:1757:MET:HG3	2.24	0.53
1:A:3232:ARG:HG2	1:A:3272:TRP:HH2	1.74	0.53
3:C:261:ILE:HA	3:C:367:ALA:H	1.74	0.53
1:A:74:ASN:HB3	1:A:121:ALA:HA	1.90	0.53
1:A:2288:TYR:HB2	1:A:2299:TYR:CE2	2.44	0.53
1:A:2443:MET:O	1:A:2445:LYS:N	2.41	0.53
3:C:13:CYS:HB3	3:C:59:PHE:HE2	1.73	0.53
3:C:69:SER:O	3:C:74:TYR:N	2.34	0.53
1:A:1038:LYS:HB2	1:A:1088:GLU:OE2	2.08	0.53
1:A:1086:TYR:CE2	1:A:1087:ARG:HD2	2.44	0.53
1:A:1098:GLN:HB3	1:A:1099:PHE:HD1	1.74	0.53
1:A:1115:HIS:CG	1:A:1180:GLN:HA	2.43	0.53
1:A:1723:PRO:HG2	1:A:1729:PHE:HZ	1.73	0.53
2:B:38:LEU:O	2:B:83:LEU:HD23	2.09	0.53
2:B:288:LEU:HD13	3:C:313:GLY:H	1.72	0.53
2:B:413:LEU:HG	2:B:432:PHE:CD1	2.44	0.53
2:B:469:LEU:HB2	2:B:517:ARG:NH2	2.24	0.53
1:A:1206:LEU:HG	1:A:1209:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1528:LEU:O	1:A:1532:LEU:N	2.42	0.53
1:A:1575:LEU:HD23	1:A:1575:LEU:H	1.74	0.53
1:A:1920:TYR:HA	1:A:1923:PHE:HB3	1.90	0.53
1:A:2155:GLU:H	1:A:2155:GLU:CD	2.16	0.53
1:A:2185:MET:SD	1:A:2186:VAL:N	2.82	0.53
4:D:25:DA:H2"	4:D:26:DA:C8	2.44	0.53
1:A:261:ASP:O	1:A:264:ARG:NH2	2.42	0.53
1:A:1018:VAL:HG12	1:A:1074:LYS:HA	1.90	0.53
1:A:1158:PRO:HG2	1:A:1159:PRO:HD3	1.90	0.53
1:A:2220:MET:HA	1:A:2223:VAL:HG12	1.90	0.53
1:A:3292:GLY:HA2	1:A:3348:LEU:HD13	1.90	0.53
1:A:3304:VAL:HA	1:A:3308:ASP:OD1	2.09	0.53
1:A:3822:GLN:H	1:A:3822:GLN:CD	2.16	0.53
1:A:3822:GLN:NE2	1:A:3823:GLU:OE1	2.41	0.53
1:A:3860:LYS:HE2	1:A:4073:ALA:HB2	1.91	0.53
1:A:4125:GLU:OE1	1:A:4127:TRP:NE1	2.41	0.53
2:B:356:LEU:HG	2:B:357:LYS:H	1.74	0.53
3:C:234:LEU:HD21	3:C:483:PRO:HD3	1.91	0.53
3:C:497:ARG:HH12	3:C:501:PRO:HA	1.74	0.53
1:A:433:PRO:HA	1:A:436:GLU:OE2	2.08	0.53
1:A:970:LEU:HD12	1:A:1011:GLU:HG3	1.91	0.53
1:A:1569:THR:HG22	1:A:1573:LYS:HE2	1.90	0.53
1:A:2291:GLN:OE1	1:A:2291:GLN:N	2.41	0.53
1:A:3274:VAL:HA	1:A:3277:VAL:HG12	1.91	0.53
1:A:3516:HIS:O	1:A:3516:HIS:ND1	2.37	0.53
1:A:3599:THR:O	1:A:3602:ASN:ND2	2.41	0.53
3:C:40:MET:HA	3:C:43:GLN:HG3	1.91	0.53
1:A:165:LYS:NZ	1:A:167:PRO:O	2.29	0.52
1:A:1071:ASN:OD1	1:A:1072:ALA:N	2.41	0.52
1:A:1115:HIS:CE1	1:A:1181:THR:H	2.27	0.52
1:A:1364:CYS:O	1:A:1368:LEU:HB3	2.09	0.52
1:A:1829:TRP:HB3	1:A:1830:HIS:CE1	2.44	0.52
1:A:2571:ASP:HA	1:A:2574:ASN:OD1	2.09	0.52
1:A:3812:LEU:HD23	1:A:3925:LEU:HD22	1.91	0.52
1:A:1007:VAL:HA	1:A:1010:LEU:HB3	1.91	0.52
1:A:1911:LEU:O	1:A:1914:THR:HG22	2.09	0.52
1:A:1919:CYS:O	1:A:1923:PHE:CB	2.57	0.52
1:A:2227:LYS:HZ2	1:A:2228:ARG:N	2.07	0.52
1:A:3100:LYS:HD3	1:A:3142:ILE:HG21	1.91	0.52
1:A:3421:ASP:OD1	1:A:3467:ARG:NE	2.37	0.52
1:A:3588:TRP:CE2	1:A:3609:MET:HE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4008:GLU:OE1	1:A:4010:SER:N	2.31	0.52
1:A:1672:PHE:O	1:A:1676:ILE:HG12	2.08	0.52
1:A:1711:ARG:HH22	1:A:1757:MET:HG3	1.73	0.52
1:A:3286:CYS:O	1:A:3288:SER:N	2.41	0.52
3:C:408:ALA:HA	3:C:420:VAL:O	2.10	0.52
3:C:544:LYS:NZ	3:C:546:ASP:OD2	2.43	0.52
1:A:1004:GLN:O	1:A:1007:VAL:HG12	2.10	0.52
1:A:1322:THR:HG22	1:A:1324:PRO:HD2	1.91	0.52
1:A:1640:GLU:HA	1:A:1643:MET:HE2	1.91	0.52
1:A:1807:LYS:NZ	1:A:1808:ASP:OD1	2.34	0.52
1:A:3020:ASP:N	1:A:3020:ASP:OD1	2.42	0.52
1:A:3354:ASP:HA	1:A:3357:ARG:HB2	1.90	0.52
1:A:3701:ILE:O	1:A:3704:GLN:HG3	2.10	0.52
2:B:261:LEU:HA	2:B:345:LEU:HB2	1.92	0.52
3:C:130:ARG:NH2	3:C:158:ASP:HB2	2.24	0.52
3:C:414:HIS:NE2	3:C:415:ASN:OD1	2.42	0.52
1:A:436:GLU:HB2	1:A:482:VAL:HG22	1.92	0.52
1:A:3180:ASP:OD1	1:A:3181:ASP:N	2.42	0.52
3:C:109:ASP:HA	3:C:112:ILE:HG12	1.91	0.52
3:C:209:LYS:HA	3:C:212:MET:HG3	1.92	0.52
5:E:29:DG:H2"	5:E:30:DT:H5"	1.90	0.52
1:A:67:VAL:HA	1:A:70:ARG:CZ	2.39	0.52
1:A:227:LEU:O	1:A:230:LEU:N	2.37	0.52
1:A:537:SER:O	1:A:561:ASN:ND2	2.42	0.52
3:C:197:ILE:HD12	3:C:201:GLN:HB2	1.90	0.52
3:C:549:THR:O	3:C:551:GLN:NE2	2.42	0.52
1:A:76:ILE:HA	1:A:79:ARG:HB2	1.92	0.52
1:A:1093:GLU:O	1:A:1095:LEU:N	2.43	0.52
1:A:1203:SER:OG	1:A:1205:ASN:OD1	2.27	0.52
1:A:1439:PRO:O	1:A:1442:GLN:NE2	2.41	0.52
1:A:1479:VAL:HG11	1:A:1518:ALA:HA	1.91	0.52
1:A:2089:ASN:OD1	1:A:2090:ARG:N	2.43	0.52
1:A:2217:ASN:HA	1:A:2220:MET:HE3	1.91	0.52
1:A:2329:TYR:O	1:A:2331:MET:N	2.42	0.52
1:A:3731:SER:OG	1:A:3732:LEU:N	2.42	0.52
1:A:105:VAL:HG13	1:A:148:LYS:HZ1	1.74	0.52
1:A:138:PHE:HE2	1:A:177:LEU:HG	1.75	0.52
1:A:351:ASN:OD1	1:A:352:VAL:N	2.43	0.52
2:B:49:PHE:CE2	2:B:132:GLN:HG2	2.45	0.52
1:A:1497:ARG:HH12	1:A:1539:SER:HB3	1.75	0.52
1:A:2239:LYS:O	1:A:2243:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3290:SER:O	1:A:3294:SER:OG	2.24	0.52
1:A:3659:PHE:HA	1:A:3662:ILE:HD13	1.91	0.52
2:B:214:SER:HB3	2:B:218:ARG:HD3	1.91	0.52
2:B:343:PRO:HA	2:B:401:THR:OG1	2.10	0.52
1:A:234:PHE:HB2	1:A:236:LYS:HZ2	1.75	0.52
1:A:280:SER:O	1:A:283:SER:OG	2.21	0.52
1:A:3107:ILE:HG22	1:A:3111:MET:HE1	1.91	0.52
1:A:3169:PRO:HD3	1:A:3182:ILE:HD11	1.90	0.52
1:A:4018:GLN:O	1:A:4022:LYS:NZ	2.32	0.52
1:A:147:PHE:CE2	1:A:148:LYS:HE3	2.45	0.51
1:A:200:PHE:O	1:A:204:LEU:HG	2.11	0.51
1:A:257:ARG:NH1	1:A:261:ASP:HB3	2.25	0.51
1:A:542:ASP:N	1:A:542:ASP:OD1	2.41	0.51
1:A:1395:LEU:HB3	1:A:1396:PRO:HD3	1.91	0.51
2:B:76:ILE:HD12	2:B:248:ALA:HA	1.92	0.51
1:A:1359:LEU:H	1:A:1361:LYS:HG2	1.74	0.51
1:A:1784:ARG:HB2	1:A:1784:ARG:HH11	1.74	0.51
1:A:2462:VAL:N	1:A:2473:MET:HE1	2.24	0.51
1:A:2773:ARG:HG3	1:A:2775:TYR:CE2	2.46	0.51
1:A:3313:SER:O	1:A:3316:LEU:HG	2.10	0.51
1:A:869:ASN:O	1:A:872:THR:OG1	2.28	0.51
1:A:877:ASP:O	1:A:881:LYS:HG2	2.10	0.51
1:A:1166:LEU:O	1:A:1170:LYS:HG2	2.09	0.51
1:A:3019:ILE:HG21	1:A:3030:ILE:HD12	1.91	0.51
2:B:441:ASP:OD1	2:B:441:ASP:N	2.43	0.51
1:A:346:TYR:HA	1:A:349:ILE:HG12	1.91	0.51
1:A:801:LYS:HD3	1:A:3114:TYR:CE2	2.45	0.51
3:C:144:LYS:HZ2	3:C:147:LEU:HD11	1.75	0.51
1:A:976:VAL:O	1:A:981:ARG:NH2	2.43	0.51
1:A:3603:LYS:HA	1:A:3606:ILE:HG12	1.93	0.51
1:A:3814:ASP:O	1:A:3818:ASN:HB2	2.10	0.51
2:B:152:ASN:O	2:B:155:SER:OG	2.26	0.51
2:B:281:LEU:HD23	2:B:281:LEU:H	1.75	0.51
3:C:20:MET:HB2	3:C:31:PHE:HB2	1.93	0.51
3:C:153:SER:O	3:C:157:CYS:N	2.43	0.51
3:C:283:THR:HG23	3:C:285:LYS:H	1.75	0.51
1:A:545:LEU:HA	1:A:548:GLU:CD	2.35	0.51
1:A:876:SER:OG	1:A:876:SER:O	2.29	0.51
1:A:936:SER:OG	1:A:2773:ARG:NH1	2.43	0.51
2:B:213:ILE:HG22	2:B:214:SER:N	2.26	0.51
2:B:264:ASN:OD1	2:B:267:ILE:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:137:ASP:N	3:C:137:ASP:OD1	2.44	0.51
1:A:3003:ASN:OD1	1:A:3046:ARG:NH2	2.39	0.51
1:A:3059:GLN:OE1	1:A:3062:LEU:HD23	2.11	0.51
1:A:3459:ASN:HB2	1:A:3462:ARG:HH21	1.75	0.51
1:A:3585:PHE:CZ	1:A:3666:LEU:HD22	2.46	0.51
1:A:4096:SER:OG	1:A:4097:GLY:N	2.44	0.51
2:B:95:ASN:OD1	2:B:98:ASN:N	2.44	0.51
1:A:183:GLU:O	1:A:185:HIS:ND1	2.43	0.51
1:A:303:HIS:CG	1:A:304:THR:H	2.28	0.51
1:A:390:GLN:HA	1:A:393:LYS:HZ3	1.75	0.51
1:A:888:ARG:HB3	1:A:3889:ARG:NH2	2.25	0.51
1:A:1069:HIS:CG	1:A:1074:LYS:HD2	2.45	0.51
1:A:1326:GLU:O	1:A:1329:ARG:HB3	2.11	0.51
1:A:3173:MET:HE2	1:A:3173:MET:HA	1.92	0.51
1:A:4016:PHE:O	1:A:4020:MET:HG3	2.11	0.51
2:B:202:LEU:O	2:B:203:MET:HE2	2.11	0.51
2:B:463:LYS:HG3	3:C:383:ALA:HB1	1.92	0.51
3:C:69:SER:O	3:C:73:GLN:N	2.44	0.51
3:C:142:PHE:HZ	3:C:200:GLN:HE22	1.57	0.51
1:A:994:TRP:CD2	1:A:2581:LEU:HD13	2.46	0.51
4:D:37:DT:H2'	4:D:38:DT:C4	2.45	0.51
1:A:86:LEU:HB3	1:A:129:ASP:HB3	1.93	0.51
1:A:785:MET:N	1:A:785:MET:SD	2.83	0.51
1:A:1666:GLY:O	1:A:1668:PHE:N	2.42	0.51
1:A:1716:GLN:HA	1:A:1719:VAL:HG22	1.93	0.51
1:A:2161:ALA:O	1:A:2165:LEU:N	2.44	0.51
1:A:2257:PHE:HA	1:A:2260:PHE:CE2	2.45	0.51
2:B:448:PHE:HA	3:C:416:TYR:OH	2.11	0.51
1:A:1382:ILE:HG21	1:A:1395:LEU:HD12	1.92	0.50
1:A:1685:ASP:OD1	1:A:1685:ASP:N	2.44	0.50
1:A:1709:GLU:HG3	1:A:1712:ARG:HH22	1.75	0.50
1:A:1709:GLU:HG3	1:A:1712:ARG:NH2	2.26	0.50
1:A:1800:SER:O	1:A:1804:MET:HE1	2.11	0.50
1:A:1900:PHE:HB2	1:A:1911:LEU:HD22	1.93	0.50
1:A:1925:GLU:HB2	1:A:1941:HIS:HE2	1.75	0.50
2:B:418:GLU:HB2	2:B:430:PRO:HB3	1.93	0.50
3:C:186:GLY:O	3:C:228:SER:HB2	2.11	0.50
3:C:513:TRP:O	3:C:517:ASN:N	2.44	0.50
1:A:1323:SER:OG	1:A:1324:PRO:HD3	2.11	0.50
1:A:1804:MET:HB2	1:A:1811:ARG:HH22	1.76	0.50
1:A:2164:TRP:C	1:A:2167:PRO:HD2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:PHE:HB2	1:A:901:MET:O	2.10	0.50
1:A:1173:LEU:HA	1:A:1176:CYS:HB2	1.94	0.50
1:A:2094:MET:HE1	1:A:2145:PHE:CE2	2.46	0.50
1:A:3347:CYS:C	1:A:3349:ALA:H	2.20	0.50
1:A:1649:LEU:O	1:A:1652:ILE:HG22	2.12	0.50
1:A:3064:PHE:O	1:A:3068:ALA:CB	2.60	0.50
1:A:3650:LYS:HD2	1:A:3653:ARG:HD3	1.92	0.50
1:A:95:LYS:HZ2	1:A:100:ILE:HB	1.77	0.50
1:A:780:ILE:HG13	1:A:785:MET:SD	2.52	0.50
1:A:1270:PHE:O	1:A:1275:THR:HB	2.11	0.50
1:A:2452:ARG:HH21	1:A:2494:ASP:CG	2.18	0.50
1:A:2821:ASP:HB2	1:A:2822:LYS:NZ	2.27	0.50
1:A:2473:MET:O	1:A:2477:LEU:HG	2.11	0.50
1:A:3820:MET:HE1	1:A:3824:GLU:C	2.37	0.50
1:A:4055:ASN:HB3	1:A:4058:VAL:HG23	1.94	0.50
2:B:322:TYR:CE2	3:C:47:PHE:HA	2.44	0.50
2:B:350:PHE:HB3	2:B:394:VAL:HG22	1.92	0.50
1:A:240:GLU:HB2	1:A:242:PRO:HD2	1.94	0.50
1:A:257:ARG:NH1	1:A:261:ASP:O	2.44	0.50
1:A:1324:PRO:HB2	1:A:1325:GLN:CD	2.37	0.50
1:A:1504:ASP:OD1	1:A:1505:LEU:N	2.42	0.50
1:A:1881:TYR:HB3	1:A:1954:CYS:SG	2.52	0.50
1:A:1986:ARG:HA	1:A:2184:TYR:HD2	1.77	0.50
1:A:2251:ILE:HD12	1:A:2251:ILE:H	1.77	0.50
1:A:71:LYS:HZ2	1:A:78:PHE:HE2	1.58	0.50
1:A:1435:ASN:OD1	1:A:1436:LEU:N	2.44	0.50
1:A:2446:LEU:HD23	1:A:2451:LEU:HD13	1.92	0.50
1:A:2828:GLU:O	1:A:2832:ILE:HG12	2.11	0.50
1:A:3638:LYS:O	1:A:3642:LYS:HG2	2.12	0.50
2:B:287:LYS:O	2:B:295:PRO:HA	2.12	0.50
1:A:135:LEU:HA	1:A:138:PHE:CD2	2.47	0.50
1:A:191:ASN:OD1	1:A:192:ASN:N	2.45	0.50
1:A:962:TYR:HA	1:A:965:THR:HG22	1.93	0.50
1:A:1140:LYS:HD2	1:A:1141:LYS:NZ	2.27	0.50
1:A:1413:ASP:O	1:A:1417:THR:HG23	2.12	0.50
1:A:1959:LEU:HA	1:A:1961:PHE:CE2	2.47	0.50
1:A:2234:ASN:HA	1:A:2237:ILE:HD12	1.94	0.50
1:A:2579:HIS:N	1:A:2784:GLN:OE1	2.45	0.49
1:A:3589:SER:O	1:A:3593:ARG:HG2	2.12	0.49
2:B:147:LEU:HD12	2:B:193:LEU:HD12	1.93	0.49
3:C:390:VAL:HG12	3:C:409:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:ILE:HD12	1:A:1558:TYR:HD2	1.77	0.49
1:A:3190:LEU:HB3	1:A:3231:ILE:HG23	1.93	0.49
1:A:87:LYS:O	1:A:91:ILE:HG12	2.12	0.49
1:A:89:LEU:C	1:A:133:LYS:HZ3	2.21	0.49
1:A:237:SER:O	1:A:238:MET:HE2	2.11	0.49
1:A:1526:GLU:CD	1:A:1526:GLU:H	2.21	0.49
1:A:2120:ARG:HB3	1:A:2160:TYR:CE2	2.48	0.49
1:A:2306:ASN:HA	1:A:2309:PHE:CE2	2.48	0.49
1:A:2307:MET:SD	1:A:2308:SER:N	2.85	0.49
1:A:3499:ILE:HA	1:A:3502:MET:HE3	1.94	0.49
3:C:411:HIS:HB3	3:C:418:CYS:SG	2.52	0.49
4:D:35:DT:C4	4:D:36:DA:C6	3.00	0.49
1:A:1389:VAL:C	1:A:1391:VAL:N	2.70	0.49
1:A:1664:SER:HA	1:A:1668:PHE:CE1	2.48	0.49
1:A:1733:THR:HB	1:A:1736:PHE:HB2	1.93	0.49
1:A:3100:LYS:O	1:A:3103:ILE:HG22	2.13	0.49
1:A:3658:ASP:O	1:A:3662:ILE:HD12	2.12	0.49
1:A:3726:VAL:HG22	1:A:3738:ILE:HG22	1.94	0.49
2:B:46:LYS:HA	2:B:49:PHE:CD1	2.47	0.49
3:C:354:ARG:HG3	3:C:355:PHE:CD1	2.46	0.49
3:C:536:LEU:HD22	3:C:537:PHE:CZ	2.47	0.49
1:A:35:ILE:HG21	1:A:80:GLU:HG3	1.94	0.49
1:A:1298:LEU:HD12	1:A:1367:HIS:HB3	1.94	0.49
1:A:1786:ALA:HB2	1:A:1827:LEU:HD12	1.95	0.49
1:A:3857:LEU:HA	1:A:3860:LYS:HE3	1.95	0.49
3:C:508:ILE:HD13	3:C:513:TRP:HE1	1.77	0.49
3:C:510:GLN:OE1	3:C:513:TRP:HB2	2.13	0.49
1:A:65:LEU:HD23	1:A:65:LEU:H	1.78	0.49
1:A:643:GLU:HG2	1:A:644:PRO:HD3	1.94	0.49
1:A:1334:LYS:O	1:A:1338:VAL:HG23	2.12	0.49
1:A:1503:LEU:HB3	1:A:1507:CYS:HB2	1.93	0.49
1:A:1669:PRO:O	1:A:1673:THR:HG23	2.12	0.49
1:A:1879:VAL:HA	1:A:1882:SER:OG	2.12	0.49
1:A:3356:ALA:HB1	1:A:3360:LEU:HB2	1.93	0.49
3:C:55:ALA:HB2	3:C:83:LEU:HD13	1.95	0.49
3:C:58:LEU:HD21	3:C:98:ILE:HD12	1.94	0.49
4:D:38:DT:H2"	4:D:39:DA:N7	2.28	0.49
1:A:1416:GLU:OE1	1:A:1420:ARG:NE	2.43	0.49
1:A:3953:LEU:HD22	1:A:4026:SER:HB3	1.95	0.49
2:B:268:VAL:HG22	3:C:539:LEU:HD23	1.95	0.49
2:B:391:GLU:OE2	2:B:392:LYS:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:GLU:OE2	3:C:428:GLU:N	2.46	0.49
3:C:538:PRO:C	3:C:539:LEU:HD12	2.38	0.49
1:A:202:GLY:O	1:A:206:THR:HG23	2.13	0.49
1:A:1684:LEU:HG	1:A:1689:LYS:HE3	1.95	0.49
1:A:3525:TYR:CE2	1:A:3712:LEU:HB2	2.48	0.49
1:A:3747:GLU:OE1	1:A:3747:GLU:N	2.45	0.49
3:C:376:ALA:O	3:C:379:SER:OG	2.30	0.49
1:A:1709:GLU:HA	1:A:1712:ARG:NH1	2.28	0.49
1:A:2397:CYS:O	1:A:2400:VAL:HG12	2.12	0.49
1:A:2428:ASP:HB3	1:A:2431:ARG:HD3	1.95	0.49
2:B:126:GLN:HA	2:B:129:LYS:HG2	1.95	0.49
1:A:2145:PHE:HD1	1:A:2146:LEU:HD22	1.78	0.49
1:A:2986:PRO:HG2	1:A:2991:LYS:HE3	1.94	0.49
2:B:87:PHE:HE1	2:B:105:LEU:HD12	1.78	0.49
2:B:349:GLY:HA3	3:C:463:LEU:HD23	1.95	0.49
2:B:533:ASP:OD1	2:B:534:TYR:N	2.44	0.49
3:C:30:PRO:HA	3:C:33:GLN:HG2	1.95	0.49
3:C:465:LYS:HB3	3:C:474:GLU:HG2	1.94	0.49
5:E:19:DA:H8	5:E:19:DA:OP2	1.96	0.49
5:E:20:DT:H2"	5:E:21:DA:C6	2.47	0.49
1:A:1202:ARG:NE	1:A:1202:ARG:HA	2.28	0.48
1:A:3580:ASN:HB3	1:A:3583:LEU:HD12	1.96	0.48
1:A:3677:PRO:HG2	1:A:3736:LYS:NZ	2.28	0.48
2:B:301:ARG:HB2	2:B:310:LEU:HD12	1.93	0.48
1:A:928:VAL:O	1:A:932:GLU:HG3	2.12	0.48
1:A:2464:HIS:O	1:A:2466:SER:N	2.46	0.48
1:A:3778:ASP:OD1	1:A:3780:ALA:N	2.46	0.48
4:D:24:DA:C6	4:D:25:DA:C6	3.02	0.48
1:A:105:VAL:HG13	1:A:148:LYS:NZ	2.28	0.48
1:A:432:THR:O	1:A:435:LEU:N	2.46	0.48
1:A:1897:ASN:N	1:A:1898:GLN:OE1	2.45	0.48
1:A:3390:GLN:O	1:A:3393:GLU:HG3	2.13	0.48
2:B:106:GLN:HG2	2:B:115:ARG:HE	1.78	0.48
1:A:66:LEU:HD13	1:A:69:VAL:HG21	1.95	0.48
1:A:747:ALA:O	1:A:750:PRO:HD2	2.12	0.48
1:A:2452:ARG:HB3	1:A:2452:ARG:NH1	2.28	0.48
2:B:450:GLU:HB2	3:C:416:TYR:HD1	1.78	0.48
2:B:515:ASN:OD1	2:B:516:LYS:N	2.43	0.48
3:C:46:VAL:HG12	3:C:86:PRO:HB2	1.96	0.48
1:A:65:LEU:C	1:A:67:VAL:H	2.22	0.48
1:A:248:ILE:O	1:A:252:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1664:SER:HA	1:A:1668:PHE:HE1	1.79	0.48
1:A:1770:GLN:OE1	1:A:1770:GLN:N	2.46	0.48
1:A:1791:CYS:O	1:A:1795:VAL:HG23	2.14	0.48
1:A:2315:VAL:HG23	1:A:2316:TYR:N	2.29	0.48
1:A:2594:ASP:OD1	1:A:2595:TRP:N	2.46	0.48
1:A:3319:ASN:OD1	1:A:3322:ALA:N	2.38	0.48
1:A:3472:ILE:CG2	1:A:3483:MET:HE3	2.20	0.48
1:A:3575:LEU:HD23	1:A:3687:MET:HE1	1.95	0.48
1:A:387:GLU:O	1:A:391:ARG:HG2	2.12	0.48
1:A:1568:ASN:O	1:A:1572:LEU:HG	2.13	0.48
1:A:1868:THR:HA	1:A:1871:MET:SD	2.54	0.48
1:A:2245:TRP:HB3	1:A:2248:CYS:HB2	1.94	0.48
1:A:2277:LEU:HA	1:A:2280:VAL:HG22	1.95	0.48
1:A:2288:TYR:CE2	1:A:2296:SER:HA	2.49	0.48
1:A:3763:ARG:HG3	1:A:4011:PHE:CE2	2.49	0.48
3:C:360:GLN:O	3:C:360:GLN:HG2	2.14	0.48
1:A:353:ASP:OD1	1:A:354:SER:N	2.47	0.48
1:A:413:PHE:O	1:A:417:VAL:HG23	2.14	0.48
1:A:446:PHE:CE1	1:A:530:LEU:HD13	2.49	0.48
1:A:681:LYS:HD3	1:A:681:LYS:N	2.29	0.48
1:A:1479:VAL:CG1	1:A:1518:ALA:HA	2.44	0.48
1:A:1857:LYS:NZ	1:A:1863:PHE:HD1	2.11	0.48
1:A:1919:CYS:O	1:A:1923:PHE:HB3	2.13	0.48
1:A:2328:ARG:CB	1:A:2370:SER:O	2.62	0.48
1:A:3324:ARG:HD2	1:A:3392:ALA:HB2	1.95	0.48
1:A:3530:VAL:O	1:A:3534:ILE:HG12	2.14	0.48
1:A:3834:ALA:O	1:A:3838:GLU:HG2	2.14	0.48
1:A:3924:HIS:CE1	1:A:3927:ASN:HD21	2.31	0.48
2:B:161:MET:HE3	2:B:161:MET:HB2	1.70	0.48
2:B:288:LEU:HD11	3:C:320:ILE:HG21	1.96	0.48
2:B:465:ILE:HD11	2:B:525:PHE:HD2	1.79	0.48
3:C:453:ALA:O	3:C:457:LEU:HD23	2.13	0.48
1:A:573:LEU:HD22	1:A:652:GLU:HG2	1.96	0.48
1:A:682:TYR:CZ	1:A:700:LYS:HG2	2.49	0.48
1:A:741:ILE:HD13	1:A:776:TRP:CZ2	2.48	0.48
1:A:849:GLU:O	1:A:853:ILE:HG12	2.14	0.48
1:A:1044:ILE:HG23	1:A:1048:GLN:HB2	1.96	0.48
1:A:1425:ALA:HB2	1:A:1467:ILE:HG22	1.95	0.48
1:A:2943:PHE:CD1	1:A:2947:ILE:HD11	2.49	0.48
3:C:88:PHE:CD1	3:C:91:LEU:HD21	2.48	0.48
1:A:186:PRO:HG2	1:A:188:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:CB	1:A:265:TYR:CE1	2.89	0.48
1:A:1133:HIS:O	1:A:1137:ILE:HG23	2.14	0.48
1:A:1557:GLU:CD	1:A:1592:MET:HE1	2.39	0.48
1:A:2207:LYS:O	1:A:2210:VAL:HG12	2.13	0.48
1:A:3840:LYS:O	1:A:3844:THR:HG23	2.14	0.48
2:B:38:LEU:HD23	2:B:39:ILE:N	2.29	0.48
2:B:452:ILE:HD11	3:C:374:ALA:HB3	1.95	0.48
3:C:199:GLU:O	3:C:202:LYS:HB2	2.14	0.48
1:A:174:VAL:O	1:A:177:LEU:HB2	2.14	0.48
1:A:1075:ARG:HD3	1:A:1113:LEU:HD23	1.95	0.48
1:A:1093:GLU:HG2	1:A:1094:SER:H	1.79	0.48
1:A:1574:ASN:HD21	1:A:1577:LEU:HD12	1.78	0.48
1:A:1624:GLN:HG3	1:A:1625:HIS:CE1	2.49	0.48
1:A:1848:ILE:HG22	1:A:1852:LYS:HE3	1.95	0.48
1:A:2383:PHE:HB3	1:A:2418:LYS:HZ3	1.79	0.48
1:A:3030:ILE:O	1:A:3034:PRO:HD3	2.14	0.48
2:B:118:GLU:O	2:B:121:GLN:HG2	2.13	0.48
2:B:143:LEU:O	2:B:146:VAL:HG22	2.14	0.48
2:B:474:ARG:NH1	2:B:474:ARG:HA	2.29	0.48
3:C:130:ARG:HH21	3:C:158:ASP:HB2	1.79	0.48
1:A:37:GLY:HA2	1:A:40:GLN:HE21	1.78	0.47
1:A:1118:GLU:N	1:A:1118:GLU:OE1	2.47	0.47
1:A:3072:GLU:HA	1:A:3075:LYS:HB2	1.96	0.47
2:B:480:ASN:HB3	3:C:428:GLU:OE2	2.14	0.47
3:C:413:LYS:NZ	3:C:416:TYR:O	2.24	0.47
1:A:1299:GLU:OE2	1:A:1304:HIS:N	2.47	0.47
1:A:3270:ASP:O	1:A:3274:VAL:HG13	2.13	0.47
1:A:3542:PHE:O	1:A:3543:LYS:HG2	2.13	0.47
1:A:3645:GLY:H	1:A:3650:LYS:NZ	2.10	0.47
2:B:240:GLU:HG2	2:B:241:ASP:N	2.29	0.47
3:C:89:ASP:O	3:C:92:GLU:HG3	2.14	0.47
3:C:461:MET:HB3	3:C:526:SER:OG	2.14	0.47
4:D:36:DA:H2'	4:D:37:DT:O4'	2.14	0.47
1:A:384:MET:CA	1:A:387:GLU:OE1	2.56	0.47
1:A:1079:SER:OG	1:A:1126:GLN:HB3	2.14	0.47
1:A:1216:GLY:O	1:A:1220:LEU:HG	2.14	0.47
1:A:1473:THR:HB	1:A:1477:HIS:CE1	2.49	0.47
1:A:1567:ILE:O	1:A:1571:LEU:HD23	2.14	0.47
1:A:3342:SER:O	1:A:3345:PRO:HD3	2.15	0.47
1:A:3496:ILE:HD12	1:A:3499:ILE:HD11	1.96	0.47
1:A:4126:PRO:HD2	1:A:4127:TRP:CZ3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:PHE:CD2	3:C:224:ILE:HG23	2.49	0.47
1:A:183:GLU:HG2	1:A:185:HIS:CE1	2.49	0.47
1:A:534:LEU:HG	1:A:564:LEU:HD13	1.96	0.47
1:A:1418:HIS:O	1:A:1421:GLU:HB2	2.14	0.47
1:A:1769:GLU:HB2	1:A:1772:HIS:CE1	2.49	0.47
1:A:2191:ALA:O	1:A:2195:SER:OG	2.30	0.47
1:A:2242:VAL:HG13	1:A:2283:ASN:HD21	1.79	0.47
1:A:2461:PHE:C	1:A:2473:MET:HE1	2.40	0.47
1:A:3180:ASP:HA	1:A:3242:MET:HE1	1.95	0.47
1:A:3644:PHE:HA	1:A:3653:ARG:NH2	2.29	0.47
2:B:91:GLU:N	2:B:91:GLU:OE1	2.48	0.47
1:A:463:LYS:HE2	1:A:544:ILE:HD12	1.96	0.47
1:A:666:PHE:O	1:A:670:LEU:N	2.36	0.47
1:A:1839:PHE:CE2	1:A:1843:ILE:HD13	2.49	0.47
1:A:1853:SER:OG	1:A:1854:ARG:N	2.42	0.47
5:E:32:DT:H2"	5:E:33:DA:N7	2.29	0.47
1:A:1142:HIS:CD2	1:A:1143:VAL:HG13	2.49	0.47
1:A:1632:TRP:N	1:A:1632:TRP:CD1	2.81	0.47
1:A:2223:VAL:O	1:A:2223:VAL:HG13	2.14	0.47
1:A:2313:LYS:HA	1:A:2316:TYR:CZ	2.49	0.47
1:A:3041:LEU:HA	1:A:3044:MET:HE2	1.97	0.47
1:A:3244:ASP:OD1	1:A:3247:ARG:NE	2.30	0.47
1:A:3384:HIS:HA	1:A:3387:GLU:OE1	2.15	0.47
1:A:3662:ILE:HA	1:A:3665:MET:HG3	1.96	0.47
1:A:3772:ASN:OD1	1:A:3788:LEU:HB2	2.15	0.47
2:B:440:ALA:HB2	3:C:481:LYS:C	2.40	0.47
3:C:280:ASP:HB3	3:C:283:THR:HG22	1.96	0.47
3:C:339:CYS:N	3:C:396:ALA:HB3	2.29	0.47
3:C:394:ARG:HH21	3:C:403:PRO:HG3	1.80	0.47
1:A:207:GLN:OE1	1:A:217:LEU:HD12	2.14	0.47
1:A:634:LEU:N	1:A:635:PRO:HD2	2.30	0.47
1:A:1155:ARG:HE	1:A:3691:LYS:HE2	1.78	0.47
1:A:1707:LEU:HD12	1:A:1707:LEU:H	1.80	0.47
1:A:1838:GLU:O	1:A:1841:SER:OG	2.27	0.47
1:A:2244:CYS:SG	1:A:2245:TRP:N	2.87	0.47
1:A:3148:GLN:CD	1:A:3148:GLN:H	2.23	0.47
1:A:3309:GLU:HG2	1:A:3310:ASN:N	2.28	0.47
1:A:3320:ILE:HG13	1:A:3391:ALA:HB1	1.97	0.47
1:A:3452:LYS:O	1:A:3455:LYS:HB3	2.14	0.47
1:A:3479:THR:HA	1:A:3483:MET:HB2	1.96	0.47
2:B:352:PRO:HB2	2:B:354:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:GLY:O	2:B:380:THR:CB	2.63	0.47
3:C:284:LEU:O	3:C:285:LYS:HD2	2.15	0.47
1:A:28:ALA:O	1:A:32:HIS:ND1	2.47	0.47
1:A:1393:ALA:C	1:A:1396:PRO:HD2	2.40	0.47
1:A:2094:MET:O	1:A:2098:THR:HG23	2.15	0.47
1:A:3503:VAL:HG11	1:A:3533:PHE:HA	1.96	0.47
1:A:3658:ASP:O	1:A:3661:ASP:HB2	2.14	0.47
1:A:3975:LYS:HE2	1:A:3975:LYS:HB3	1.68	0.47
1:A:133:LYS:HD2	1:A:133:LYS:HA	1.62	0.47
1:A:193:ALA:O	1:A:197:PHE:HD2	1.98	0.47
1:A:350:ARG:HH12	1:A:351:ASN:HB2	1.80	0.47
1:A:1223:THR:HG22	1:A:1224:PHE:CD1	2.49	0.47
1:A:1657:SER:C	1:A:1659:VAL:H	2.23	0.47
1:A:2288:TYR:CE1	1:A:2294:ILE:HD11	2.49	0.47
2:B:129:LYS:HA	2:B:132:GLN:HG3	1.97	0.47
2:B:312:LEU:O	2:B:316:THR:HG23	2.15	0.47
2:B:383:SER:O	2:B:387:ILE:HG12	2.15	0.47
1:A:1699:PHE:C	1:A:1701:SER:H	2.23	0.47
1:A:1828:LEU:HA	1:A:1831:CYS:SG	2.55	0.47
1:A:3066:ASP:O	1:A:3069:MET:HG3	2.15	0.47
1:A:3419:PHE:O	1:A:3422:GLN:HG2	2.14	0.47
2:B:169:PHE:CE1	2:B:203:MET:HG3	2.50	0.47
3:C:236:VAL:HG13	3:C:237:PHE:CD1	2.50	0.47
1:A:95:LYS:NZ	1:A:100:ILE:HB	2.30	0.46
1:A:108:LYS:HA	1:A:111:CYS:SG	2.55	0.46
1:A:984:TYR:O	1:A:987:LEU:N	2.48	0.46
1:A:1192:TYR:OH	1:A:1275:THR:OG1	2.33	0.46
1:A:1868:THR:O	1:A:1871:MET:HB2	2.15	0.46
1:A:2120:ARG:HG2	1:A:2159:PRO:HB2	1.97	0.46
1:A:2288:TYR:HB2	1:A:2299:TYR:HE2	1.79	0.46
1:A:3711:PRO:C	1:A:3712:LEU:HD22	2.41	0.46
1:A:3755:GLY:HA2	1:A:3799:ARG:O	2.15	0.46
1:A:3806:LEU:C	1:A:3807:GLU:HG3	2.40	0.46
1:A:4115:ASN:OD1	1:A:4119:ARG:NH1	2.35	0.46
2:B:184:SER:O	2:B:188:THR:HG23	2.15	0.46
2:B:372:GLU:HG2	2:B:375:VAL:O	2.15	0.46
3:C:131:HIS:ND1	3:C:160:SER:O	2.48	0.46
3:C:154:LEU:HD13	3:C:215:LEU:HD13	1.95	0.46
1:A:24:ARG:NH1	1:A:69:VAL:O	2.49	0.46
1:A:901:MET:C	1:A:902:LYS:HD2	2.40	0.46
1:A:2409:THR:OG1	1:A:2410:GLU:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3020:ASP:HB2	1:A:3022:GLU:OE1	2.16	0.46
1:A:3537:SER:HA	1:A:3540:TYR:CZ	2.50	0.46
2:B:60:PHE:O	2:B:64:ILE:HG12	2.15	0.46
2:B:176:HIS:C	2:B:178:ASN:H	2.23	0.46
2:B:279:LYS:HB3	3:C:357:MET:HE1	1.97	0.46
3:C:162:GLN:HA	3:C:223:GLU:OE2	2.15	0.46
1:A:250:ASN:C	1:A:254:LYS:HZ2	2.23	0.46
1:A:305:ASN:O	1:A:309:LYS:HG2	2.15	0.46
1:A:1150:LYS:NZ	1:A:1161:ALA:O	2.46	0.46
1:A:1484:LEU:HD12	1:A:1485:SER:N	2.30	0.46
1:A:1784:ARG:HB2	1:A:1784:ARG:NH1	2.30	0.46
1:A:2332:GLU:HB3	1:A:2335:ASN:O	2.16	0.46
1:A:2966:SER:HA	1:A:3005:LEU:HD11	1.97	0.46
1:A:3781:CYS:HB3	1:A:3786:LEU:HD12	1.95	0.46
2:B:336:GLU:HA	2:B:339:ARG:HG2	1.97	0.46
2:B:411:VAL:HB	2:B:434:LEU:HD22	1.97	0.46
3:C:164:PHE:HE1	3:C:230:SER:HB3	1.79	0.46
3:C:212:MET:HE1	3:C:223:GLU:HB3	1.97	0.46
3:C:474:GLU:OE1	3:C:474:GLU:N	2.48	0.46
3:C:526:SER:C	3:C:529:PRO:HD2	2.41	0.46
1:A:239:GLU:N	1:A:243:GLN:HE22	2.10	0.46
1:A:1920:TYR:CZ	1:A:1924:THR:HG21	2.51	0.46
1:A:2183:HIS:C	1:A:2185:MET:H	2.21	0.46
1:A:2269:ASP:CG	1:A:2270:ASN:H	2.23	0.46
1:A:4065:LEU:HD23	1:A:4065:LEU:HA	1.71	0.46
2:B:363:ARG:NH2	5:E:28:DA:OP1	2.49	0.46
3:C:81:ARG:NH2	3:C:84:MET:HG2	2.29	0.46
1:A:739:ASN:O	1:A:742:GLU:HG2	2.14	0.46
1:A:878:GLU:O	1:A:879:MET:HE2	2.16	0.46
1:A:959:TYR:O	1:A:962:TYR:HB2	2.15	0.46
1:A:1583:MET:CE	1:A:1629:CYS:HB2	2.44	0.46
1:A:1668:PHE:HA	1:A:1671:VAL:HG12	1.97	0.46
2:B:73:SER:HB2	2:B:244:ARG:NH2	2.30	0.46
2:B:532:PRO:HB3	3:C:372:ALA:HB3	1.98	0.46
1:A:697:ASP:HB3	1:A:700:LYS:HB2	1.98	0.46
1:A:787:PRO:HA	1:A:790:LYS:NZ	2.30	0.46
1:A:942:LEU:O	1:A:946:THR:HG23	2.15	0.46
1:A:1095:LEU:HD13	1:A:1099:PHE:CD1	2.51	0.46
1:A:1444:ASP:N	1:A:1447:ARG:HH21	2.14	0.46
1:A:3763:ARG:HG3	1:A:4011:PHE:HE2	1.81	0.46
2:B:376:ILE:H	3:C:540:ILE:HG12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:CYS:HB3	3:C:59:PHE:CE2	2.50	0.46
3:C:144:LYS:NZ	3:C:147:LEU:HD11	2.30	0.46
1:A:221:ALA:O	1:A:225:LYS:HG2	2.16	0.46
1:A:538:ASP:CG	1:A:539:GLN:HE21	2.22	0.46
1:A:913:ARG:NH1	1:A:916:GLU:OE1	2.49	0.46
1:A:1216:GLY:HA2	1:A:1219:PHE:HB3	1.97	0.46
1:A:1305:ASP:O	1:A:1320:ASN:ND2	2.49	0.46
1:A:1708:GLU:O	1:A:1711:ARG:HB3	2.16	0.46
1:A:2150:VAL:HA	1:A:2153:THR:OG1	2.16	0.46
1:A:3281:CYS:HB2	1:A:3329:LEU:HD13	1.98	0.46
1:A:3826:ALA:HA	1:A:3829:LEU:HG	1.97	0.46
2:B:39:ILE:HG13	2:B:84:ALA:O	2.15	0.46
2:B:71:TYR:HD2	2:B:116:ILE:HG13	1.80	0.46
3:C:238:LYS:HG3	3:C:239:LYS:HD2	1.98	0.46
4:D:21:DA:N6	5:E:34:DT:C4	2.84	0.46
1:A:1215:GLU:HG2	1:A:1219:PHE:HB2	1.98	0.46
1:A:1452:VAL:HG11	1:A:1514:LEU:HD12	1.98	0.46
1:A:3829:LEU:HD12	1:A:3830:SER:HB3	1.98	0.46
1:A:4098:LEU:HA	1:A:4098:LEU:HD23	1.66	0.46
2:B:139:SER:OG	2:B:140:ASP:N	2.48	0.46
2:B:204:HIS:HB2	2:B:237:SER:HB3	1.98	0.46
2:B:304:ASN:HA	3:C:288:ASP:O	2.16	0.46
3:C:43:GLN:HE22	3:C:491:PHE:HD2	1.64	0.46
3:C:397:TYR:HB3	3:C:401:ALA:HB3	1.97	0.46
3:C:398:ASP:CG	3:C:400:ARG:H	2.23	0.46
1:A:134:LEU:O	1:A:137:THR:OG1	2.26	0.46
1:A:197:PHE:HA	1:A:200:PHE:HD2	1.81	0.46
1:A:249:PHE:O	1:A:252:VAL:HB	2.15	0.46
1:A:1273:GLU:OE1	1:A:1275:THR:OG1	2.33	0.46
1:A:1718:ILE:HA	1:A:1722:PHE:HD2	1.81	0.46
1:A:2443:MET:C	1:A:2445:LYS:H	2.24	0.46
3:C:229:GLU:O	3:C:233:LYS:N	2.45	0.46
1:A:275:PHE:HD2	1:A:315:ALA:HB1	1.81	0.46
1:A:383:PHE:O	1:A:387:GLU:OE2	2.34	0.46
1:A:1010:LEU:HD12	1:A:1014:LEU:HB2	1.98	0.46
1:A:1374:GLN:OE1	1:A:1374:GLN:HA	2.15	0.46
1:A:1404:LYS:HD2	1:A:1404:LYS:HA	1.64	0.46
1:A:1837:ARG:HH21	1:A:1895:LYS:HB2	1.81	0.46
1:A:3472:ILE:HG23	1:A:3483:MET:HE2	1.94	0.46
1:A:3610:TYR:O	1:A:3613:MET:HG3	2.16	0.46
2:B:356:LEU:HG	2:B:357:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:347:LYS:HB3	3:C:350:GLN:HG3	1.97	0.46
1:A:396:PHE:CD2	1:A:410:MET:HE1	2.51	0.45
1:A:1004:GLN:OE1	1:A:1004:GLN:HA	2.16	0.45
1:A:1009:LEU:HG	1:A:1009:LEU:O	2.16	0.45
1:A:1093:GLU:O	1:A:1096:VAL:N	2.49	0.45
1:A:1093:GLU:OE1	1:A:1093:GLU:N	2.47	0.45
1:A:1208:LEU:HA	1:A:1211:VAL:HG22	1.98	0.45
1:A:1389:VAL:C	1:A:1391:VAL:H	2.23	0.45
1:A:2254:ARG:NH2	1:A:2293:GLY:O	2.49	0.45
1:A:2943:PHE:CE1	1:A:2947:ILE:HD11	2.51	0.45
1:A:3997:LEU:O	1:A:4001:THR:N	2.42	0.45
1:A:4040:PRO:HD2	1:A:4041:ARG:NH1	2.31	0.45
2:B:194:ARG:NH1	2:B:222:SER:OG	2.49	0.45
2:B:252:ARG:NH1	5:E:26:DT:OP1	2.50	0.45
1:A:130:LEU:O	1:A:134:LEU:HG	2.16	0.45
1:A:356:ASN:HA	1:A:406:ARG:HH22	1.81	0.45
1:A:1711:ARG:NH2	1:A:1757:MET:HG3	2.30	0.45
1:A:2202:PRO:HG3	1:A:2245:TRP:CE2	2.51	0.45
1:A:3295:GLU:HG2	1:A:3296:GLN:N	2.31	0.45
1:A:3348:LEU:H	1:A:3351:ILE:HG22	1.81	0.45
4:D:21:DA:H2''	4:D:22:DA:H8	1.80	0.45
1:A:71:LYS:HZ1	1:A:77:GLU:CD	2.25	0.45
1:A:263:LYS:HB3	1:A:265:TYR:CD1	2.50	0.45
1:A:1092:GLU:CD	1:A:1095:LEU:HD23	2.41	0.45
1:A:1248:PHE:HB2	1:A:1319:GLY:N	2.31	0.45
1:A:1359:LEU:N	1:A:1361:LYS:HG2	2.31	0.45
1:A:1651:LYS:HD3	1:A:6016:UNK:O	2.16	0.45
2:B:498:MET:CG	2:B:499:GLU:H	2.27	0.45
1:A:449:TYR:CD2	1:A:453:MET:HE1	2.51	0.45
1:A:639:ALA:O	1:A:642:PHE:N	2.49	0.45
1:A:1449:ALA:HA	1:A:1452:VAL:HG22	1.98	0.45
1:A:1887:ASP:OD1	1:A:1887:ASP:N	2.43	0.45
1:A:2269:ASP:C	1:A:2271:SER:H	2.23	0.45
2:B:469:LEU:HD21	3:C:344:GLY:HA2	1.99	0.45
5:E:34:DT:H1'	5:E:35:DT:C5	2.52	0.45
1:A:173:LYS:HD3	1:A:223:CYS:SG	2.57	0.45
1:A:2093:CYS:O	1:A:2097:LEU:HD23	2.15	0.45
1:A:2100:LEU:HG	1:A:2104:MET:CE	2.47	0.45
1:A:2275:GLN:O	1:A:2279:ILE:HG12	2.17	0.45
1:A:3170:ASP:OD1	1:A:3171:ALA:N	2.49	0.45
1:A:3573:ASN:O	1:A:3577:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3644:PHE:CZ	1:A:3650:LYS:HE3	2.52	0.45
1:A:3699:LEU:O	1:A:3719:ILE:N	2.35	0.45
1:A:3910:LEU:HD12	1:A:3910:LEU:HA	1.70	0.45
1:A:4014:LYS:N	1:A:4014:LYS:HD3	2.32	0.45
2:B:399:ARG:NH1	3:C:516:LEU:HB3	2.31	0.45
3:C:442:LYS:HB2	3:C:443:LYS:NZ	2.31	0.45
1:A:537:SER:OG	1:A:541:MET:HE1	2.16	0.45
1:A:762:TYR:CD2	1:A:765:LEU:HG	2.52	0.45
1:A:1202:ARG:HD3	1:A:1206:LEU:CD2	2.46	0.45
1:A:1497:ARG:NH1	1:A:1539:SER:HB3	2.32	0.45
1:A:2145:PHE:CE1	1:A:2149:LEU:HD11	2.51	0.45
1:A:2980:ASP:OD1	1:A:2980:ASP:N	2.49	0.45
1:A:3019:ILE:HD13	1:A:3030:ILE:HD11	1.99	0.45
1:A:3285:HIS:HE1	1:A:3333:THR:HA	1.81	0.45
1:A:3542:PHE:O	1:A:3544:ASP:N	2.50	0.45
1:A:3542:PHE:C	1:A:3544:ASP:H	2.24	0.45
1:A:3645:GLY:C	1:A:3646:LYS:HD2	2.41	0.45
1:A:3754:GLY:O	1:A:3756:GLU:N	2.47	0.45
1:A:4051:LEU:HD23	1:A:4051:LEU:HA	1.70	0.45
2:B:116:ILE:H	2:B:116:ILE:HD12	1.81	0.45
2:B:162:SER:OG	2:B:163:HIS:N	2.48	0.45
2:B:252:ARG:HE	3:C:431:ARG:NH1	2.14	0.45
2:B:385:LEU:C	2:B:386:LEU:HD22	2.42	0.45
1:A:392:CYS:O	1:A:396:PHE:N	2.44	0.45
1:A:425:ASP:OD1	1:A:425:ASP:N	2.38	0.45
1:A:784:VAL:O	1:A:787:PRO:HD2	2.17	0.45
1:A:876:SER:O	1:A:879:MET:N	2.47	0.45
1:A:1539:SER:HA	1:A:1552:HIS:HD1	1.82	0.45
1:A:2264:ASP:HB3	1:A:2267:SER:HB2	1.97	0.45
1:A:2896:ALA:O	1:A:2900:LEU:HD13	2.16	0.45
1:A:3506:LEU:HD23	1:A:3511:ALA:HB1	1.99	0.45
1:A:4119:ARG:HG3	1:A:4119:ARG:O	2.16	0.45
2:B:57:LEU:HD21	2:B:61:ASP:OD2	2.16	0.45
2:B:91:GLU:OE2	2:B:137:HIS:N	2.48	0.45
3:C:20:MET:HE2	3:C:31:PHE:CG	2.52	0.45
4:D:42:DA:H2	5:E:15:DA:H5'	1.80	0.45
1:A:13:LEU:HG	1:A:59:PHE:HA	1.98	0.45
1:A:327:VAL:HG23	1:A:334:HIS:HB2	1.98	0.45
1:A:339:GLN:HA	1:A:342:MET:HG3	1.98	0.45
1:A:2572:TYR:HB3	1:A:2573:PRO:HD3	1.99	0.45
1:A:3120:LEU:O	1:A:3122:HIS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3174:ASP:O	1:A:3249:GLN:NE2	2.33	0.45
1:A:3465:PHE:N	1:A:3466:PRO:HD2	2.32	0.45
1:A:3847:SER:HB3	1:A:3854:ALA:HB1	1.99	0.45
1:A:3880:ALA:HB2	1:A:3965:ARG:NH2	2.31	0.45
3:C:273:LYS:HD3	3:C:273:LYS:N	2.32	0.45
3:C:280:ASP:OD1	3:C:281:ALA:N	2.50	0.45
3:C:528:ILE:H	3:C:528:ILE:HD12	1.82	0.45
1:A:752:LEU:HD12	1:A:752:LEU:HA	1.78	0.45
1:A:1185:HIS:NE2	1:A:1265:GLU:OE1	2.47	0.45
1:A:1708:GLU:H	1:A:1708:GLU:CD	2.24	0.45
1:A:1718:ILE:HA	1:A:1722:PHE:CD2	2.52	0.45
1:A:2371:PHE:CD1	1:A:2373:PRO:HD2	2.52	0.45
1:A:2466:SER:C	1:A:2468:THR:H	2.25	0.45
1:A:3071:GLY:N	1:A:3075:LYS:HE2	2.32	0.45
1:A:3833:ARG:NE	1:A:3833:ARG:HA	2.32	0.45
2:B:303:PHE:HZ	2:B:308:GLY:HA2	1.81	0.45
3:C:216:GLU:OE2	3:C:219:ASP:HB2	2.17	0.45
3:C:287:GLU:HG2	3:C:288:ASP:H	1.82	0.45
1:A:30:ALA:HA	1:A:33:GLN:HE21	1.82	0.45
1:A:240:GLU:OE2	1:A:243:GLN:HB3	2.16	0.45
1:A:291:VAL:HA	1:A:294:PHE:HB3	1.99	0.45
1:A:345:PHE:HA	1:A:348:ILE:HG12	1.98	0.45
1:A:932:GLU:OE2	1:A:2771:LEU:HD13	2.17	0.45
1:A:1424:THR:C	1:A:1426:GLN:H	2.24	0.45
1:A:1884:LEU:HD23	1:A:1884:LEU:HA	1.75	0.45
1:A:2211:LEU:O	1:A:2215:LEU:N	2.36	0.45
1:A:2315:VAL:HG23	1:A:2316:TYR:H	1.81	0.45
1:A:2349:LEU:O	1:A:2351:GLN:N	2.47	0.45
1:A:2576:MET:HG3	1:A:2577:PHE:CD2	2.52	0.45
2:B:45:SER:H	2:B:48:MET:HE1	1.81	0.45
2:B:290:ARG:HG2	3:C:309:ASP:HA	1.98	0.45
1:A:771:ASN:OD1	1:A:854:ARG:NH2	2.50	0.44
1:A:1111:LEU:HD13	1:A:1127:CYS:CB	2.47	0.44
1:A:1299:GLU:CD	1:A:1303:MET:HE3	2.41	0.44
1:A:1404:LYS:HD3	1:A:1461:ALA:HA	1.99	0.44
1:A:1725:GLN:OE1	1:A:1726:SER:N	2.50	0.44
1:A:2122:LEU:HD21	1:A:2163:HIS:HB3	1.98	0.44
1:A:4014:LYS:O	1:A:4015:ASN:C	2.59	0.44
3:C:16:VAL:HA	3:C:20:MET:HE3	1.99	0.44
4:D:22:DA:C2	4:D:23:DT:C2	3.05	0.44
5:E:21:DA:H2"	5:E:22:DG:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:PHE:C	1:A:553:VAL:H	2.24	0.44
1:A:623:PHE:HE2	1:A:665:GLY:HA3	1.83	0.44
1:A:850:GLU:H	1:A:850:GLU:CD	2.20	0.44
1:A:1278:ALA:O	1:A:1282:LEU:HD23	2.17	0.44
1:A:3026:ASP:OD1	1:A:3026:ASP:N	2.48	0.44
1:A:3822:GLN:HE21	1:A:3823:GLU:CD	2.25	0.44
1:A:4013:TRP:HD1	1:A:4014:LYS:HD3	1.83	0.44
2:B:59:PRO:HA	2:B:62:MET:HE3	1.98	0.44
2:B:168:LEU:HB3	2:B:202:LEU:HD12	1.99	0.44
2:B:193:LEU:HD22	2:B:198:ILE:HD12	1.98	0.44
2:B:290:ARG:HG2	3:C:309:ASP:C	2.42	0.44
1:A:1105:VAL:HG22	1:A:1171:TRP:CZ3	2.53	0.44
1:A:1150:LYS:HD2	1:A:1162:SER:HA	1.98	0.44
1:A:1406:LEU:HA	1:A:1406:LEU:HD23	1.80	0.44
1:A:1577:LEU:HD23	1:A:1580:LEU:HD12	2.00	0.44
1:A:1685:ASP:OD2	1:A:1687:HIS:HB3	2.16	0.44
1:A:3297:VAL:O	1:A:3300:VAL:HG12	2.17	0.44
2:B:95:ASN:HD21	2:B:99:PHE:H	1.65	0.44
4:D:20:DT:H2'	5:E:36:DA:C2	2.53	0.44
4:D:43:DT:H2''	4:D:44:DG:C8	2.51	0.44
1:A:1038:LYS:O	1:A:1039:TRP:HB2	2.18	0.44
1:A:1773:VAL:N	1:A:1775:GLU:OE2	2.33	0.44
1:A:1977:ILE:HG13	1:A:1978:PHE:H	1.81	0.44
1:A:2548:PRO:HB2	1:A:2848:PHE:CD1	2.52	0.44
2:B:174:ASN:OD1	2:B:174:ASN:N	2.50	0.44
2:B:356:LEU:HD23	2:B:356:LEU:H	1.81	0.44
2:B:409:TYR:HA	2:B:439:PHE:HZ	1.82	0.44
3:C:147:LEU:HD23	3:C:150:ILE:HD11	1.99	0.44
1:A:157:TYR:O	1:A:161:ALA:CB	2.66	0.44
1:A:886:TRP:HA	1:A:964:ARG:HH12	1.80	0.44
1:A:923:ASP:C	1:A:925:GLN:H	2.24	0.44
1:A:2396:LEU:O	1:A:2399:GLU:HG3	2.17	0.44
1:A:2812:LEU:HD23	1:A:2812:LEU:HA	1.86	0.44
1:A:2917:PRO:C	1:A:2919:ASP:H	2.26	0.44
1:A:3050:LYS:HD3	1:A:3050:LYS:HA	1.78	0.44
2:B:121:GLN:HG3	2:B:130:ARG:NH2	2.33	0.44
2:B:269:ILE:HA	2:B:375:VAL:HG11	1.99	0.44
2:B:329:LEU:HD21	3:C:497:ARG:HG2	1.98	0.44
1:A:13:LEU:O	1:A:17:GLU:HG2	2.17	0.44
1:A:172:GLU:OE1	1:A:172:GLU:HA	2.18	0.44
1:A:261:ASP:C	1:A:264:ARG:HH21	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HA	1:A:436:GLU:CD	2.43	0.44
1:A:1153:LEU:HD12	1:A:1154:PRO:HD2	2.00	0.44
1:A:1260:LEU:O	1:A:1264:LEU:HD23	2.17	0.44
1:A:1733:THR:HG22	1:A:1735:ARG:H	1.83	0.44
1:A:2255:LEU:O	1:A:2259:LYS:HG2	2.17	0.44
1:A:2294:ILE:C	1:A:2296:SER:H	2.26	0.44
1:A:2514:ASN:OD1	1:A:2517:LEU:N	2.48	0.44
1:A:2972:TYR:O	1:A:2976:LEU:N	2.36	0.44
1:A:3645:GLY:O	1:A:3646:LYS:HD2	2.17	0.44
1:A:3744:ASP:O	1:A:3746:ARG:HG3	2.17	0.44
1:A:3788:LEU:HD23	1:A:3788:LEU:HA	1.69	0.44
2:B:77:SER:HA	2:B:249:LYS:O	2.18	0.44
2:B:317:LYS:N	3:C:279:VAL:O	2.40	0.44
2:B:488:ARG:NE	2:B:501:GLU:HB3	2.33	0.44
3:C:64:THR:HB	3:C:66:ASN:OD1	2.18	0.44
3:C:232:ARG:HE	3:C:233:LYS:NZ	2.15	0.44
1:A:157:TYR:O	1:A:161:ALA:HB2	2.17	0.44
1:A:169:THR:HA	5:E:21:DA:H5'	2.00	0.44
1:A:267:VAL:N	1:A:268:PRO:HD2	2.32	0.44
1:A:957:PRO:C	1:A:959:TYR:H	2.25	0.44
1:A:1089:PHE:HZ	1:A:1099:PHE:HB2	1.83	0.44
1:A:1190:LEU:HD23	1:A:1190:LEU:HA	1.73	0.44
1:A:3298:LEU:HD21	1:A:3336:ILE:HB	1.99	0.44
1:A:3562:LEU:HB2	1:A:3564:GLN:HE21	1.82	0.44
1:A:3622:ALA:N	1:A:3625:LEU:HD23	2.33	0.44
1:A:3672:LYS:C	1:A:3674:SER:N	2.70	0.44
1:A:3843:LEU:HD12	1:A:3843:LEU:HA	1.86	0.44
2:B:256:LEU:HD12	2:B:256:LEU:HA	1.75	0.44
2:B:303:PHE:HD1	2:B:310:LEU:HD13	1.83	0.44
2:B:371:GLU:OE2	2:B:372:GLU:N	2.51	0.44
1:A:79:ARG:HE	1:A:126:PRO:CB	2.30	0.44
1:A:266:ALA:HA	1:A:269:SER:CB	2.48	0.44
1:A:1009:LEU:HD21	1:A:1059:LEU:HD13	2.00	0.44
1:A:1309:ALA:O	1:A:1311:LYS:HG2	2.17	0.44
1:A:1649:LEU:HD12	1:A:1649:LEU:HA	1.83	0.44
1:A:2086:ASP:HA	1:A:2089:ASN:HD21	1.83	0.44
1:A:2138:VAL:HB	1:A:2139:PRO:HD3	1.93	0.44
1:A:3424:LEU:HD21	1:A:3442:TYR:HB2	1.99	0.44
1:A:4121:TRP:CD1	1:A:4123:GLY:H	2.35	0.44
2:B:418:GLU:OE2	2:B:426:GLN:NE2	2.51	0.44
1:A:33:GLN:NE2	1:A:34:LEU:HG	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:HA	1:A:66:LEU:HD23	2.00	0.44
1:A:1273:GLU:O	1:A:1275:THR:N	2.50	0.44
1:A:1428:ILE:H	1:A:1428:ILE:HD12	1.82	0.44
1:A:1872:GLY:O	1:A:1876:ILE:N	2.50	0.44
1:A:3280:TYR:CE1	1:A:3304:VAL:HG21	2.52	0.44
1:A:111:CYS:HB2	1:A:130:LEU:CD1	2.48	0.43
1:A:1713:VAL:HA	1:A:1716:GLN:CD	2.42	0.43
1:A:2252:PRO:C	1:A:2254:ARG:H	2.25	0.43
1:A:2266:ASN:OD1	1:A:2266:ASN:N	2.51	0.43
1:A:2472:GLN:O	1:A:2476:ILE:HG12	2.17	0.43
1:A:3526:PRO:C	1:A:3528:ALA:H	2.26	0.43
2:B:298:THR:HG22	2:B:300:THR:OG1	2.17	0.43
3:C:127:PHE:CZ	3:C:130:ARG:HD3	2.53	0.43
3:C:163:PHE:HE2	3:C:165:LEU:HB2	1.82	0.43
3:C:301:ASP:OD1	3:C:302:GLU:N	2.51	0.43
1:A:294:PHE:O	1:A:298:LEU:HD23	2.18	0.43
1:A:374:LYS:HA	1:A:374:LYS:HD2	1.76	0.43
1:A:391:ARG:O	1:A:395:MET:N	2.51	0.43
1:A:881:LYS:C	1:A:883:TYR:N	2.76	0.43
1:A:1207:TRP:CH2	1:A:1211:VAL:HG11	2.53	0.43
1:A:1324:PRO:HB2	1:A:1325:GLN:NE2	2.32	0.43
1:A:1362:ASP:OD1	1:A:1363:LEU:N	2.51	0.43
1:A:2434:VAL:O	1:A:2438:ILE:HG13	2.18	0.43
1:A:3226:ASP:N	1:A:3229:SER:OG	2.51	0.43
1:A:3394:GLU:OE2	1:A:3396:ALA:N	2.51	0.43
1:A:3614:TYR:CE1	1:A:3640:PHE:HZ	2.36	0.43
2:B:126:GLN:O	2:B:130:ARG:HG2	2.18	0.43
2:B:183:ALA:HB1	2:B:187:ARG:HH12	1.82	0.43
1:A:2828:GLU:HG2	1:A:2829:LYS:N	2.33	0.43
1:A:3263:HIS:O	1:A:3266:SER:HB3	2.19	0.43
1:A:3324:ARG:HG3	1:A:3391:ALA:HB3	1.99	0.43
1:A:3669:LYS:C	1:A:3671:ASN:N	2.70	0.43
1:A:3796:MET:HE2	1:A:3796:MET:HA	2.01	0.43
2:B:484:GLN:O	2:B:488:ARG:HG3	2.18	0.43
3:C:251:LEU:N	3:C:259:ILE:O	2.51	0.43
5:E:31:DT:H2"	5:E:32:DT:OP2	2.16	0.43
1:A:172:GLU:HA	1:A:174:VAL:HG22	2.00	0.43
1:A:1069:HIS:CE1	1:A:1074:LYS:HD2	2.53	0.43
1:A:1202:ARG:HG3	1:A:1207:TRP:HD1	1.84	0.43
1:A:2479:TRP:O	1:A:2482:ASP:HB2	2.18	0.43
1:A:2551:GLU:OE1	1:A:2851:PHE:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2586:PHE:CE1	1:A:2782:ASP:HB3	2.53	0.43
1:A:3134:ALA:O	1:A:3138:ILE:HG12	2.18	0.43
1:A:3731:SER:O	1:A:3734:ARG:HD2	2.19	0.43
3:C:29:SER:O	3:C:32:GLU:HG2	2.17	0.43
1:A:1044:ILE:HD13	1:A:1044:ILE:HA	1.90	0.43
1:A:1086:TYR:O	1:A:1087:ARG:HB2	2.19	0.43
1:A:1250:LEU:O	1:A:1254:LEU:HD23	2.19	0.43
1:A:1601:LEU:HD23	1:A:1618:LEU:HD21	1.99	0.43
1:A:1681:ASP:OD2	1:A:1683:LYS:N	2.51	0.43
1:A:2291:GLN:HG2	1:A:2292:CYS:H	1.82	0.43
1:A:3464:LYS:HG2	1:A:4000:ASN:ND2	2.34	0.43
2:B:104:VAL:O	2:B:105:LEU:HD23	2.19	0.43
2:B:252:ARG:O	3:C:433:TYR:HE1	2.01	0.43
3:C:531:SER:HA	3:C:534:LYS:HE3	2.00	0.43
1:A:632:GLU:OE1	1:A:632:GLU:N	2.51	0.43
1:A:782:ARG:NH1	1:A:782:ARG:O	2.52	0.43
1:A:1082:PHE:HD1	1:A:1085:ILE:HD11	1.83	0.43
1:A:1150:LYS:HD2	1:A:1150:LYS:HA	1.82	0.43
1:A:1636:ASP:OD1	1:A:1636:ASP:N	2.52	0.43
1:A:1766:LEU:HD11	1:A:1775:GLU:HG3	2.00	0.43
1:A:1891:ALA:O	1:A:1909:ASN:N	2.50	0.43
1:A:2586:PHE:HA	1:A:2777:HIS:O	2.17	0.43
1:A:2794:LEU:HD12	1:A:2794:LEU:HA	1.80	0.43
1:A:2988:GLU:HA	1:A:2991:LYS:HG2	2.00	0.43
1:A:3302:LYS:NZ	1:A:3334:TYR:OH	2.40	0.43
1:A:4115:ASN:O	1:A:4119:ARG:NH1	2.52	0.43
2:B:48:MET:HA	2:B:59:PRO:HG2	2.00	0.43
2:B:297:LYS:HB3	3:C:296:CYS:HB3	1.99	0.43
3:C:537:PHE:HA	3:C:538:PRO:HD3	1.88	0.43
1:A:117:LYS:NZ	3:C:300:ASP:HA	2.34	0.43
1:A:149:ILE:HD11	1:A:183:GLU:HB2	2.01	0.43
1:A:421:LEU:HD12	1:A:421:LEU:HA	1.86	0.43
1:A:801:LYS:HE3	1:A:3125:ARG:HH11	1.83	0.43
1:A:1668:PHE:CG	1:A:1669:PRO:HD3	2.53	0.43
1:A:1787:ARG:HG3	1:A:1830:HIS:HB3	2.01	0.43
1:A:2217:ASN:O	1:A:2220:MET:HG2	2.19	0.43
1:A:3089:LEU:O	1:A:3093:GLN:N	2.51	0.43
1:A:3605:ASN:OD1	1:A:3605:ASN:N	2.51	0.43
2:B:95:ASN:HD21	2:B:99:PHE:N	2.17	0.43
2:B:493:LEU:HD22	3:C:323:PHE:CD2	2.53	0.43
3:C:531:SER:HA	3:C:534:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:THR:C	1:A:236:LYS:HD2	2.42	0.43
1:A:325:ASN:O	1:A:329:LYS:HG2	2.19	0.43
1:A:332:GLU:C	1:A:335:LYS:HZ1	2.21	0.43
1:A:1013:ILE:HG23	1:A:1014:LEU:N	2.34	0.43
1:A:1206:LEU:O	1:A:1209:LYS:HG2	2.18	0.43
1:A:1411:TYR:O	1:A:1414:ILE:HG12	2.19	0.43
1:A:1493:PRO:HB3	1:A:1501:PRO:HD3	2.01	0.43
1:A:1519:PHE:CD1	1:A:1524:LEU:HD23	2.54	0.43
1:A:2506:LEU:HD23	1:A:2506:LEU:HA	1.76	0.43
1:A:2857:CYS:O	1:A:2861:ILE:HG13	2.19	0.43
1:A:3271:ASP:O	1:A:3274:VAL:HG22	2.18	0.43
1:A:3599:THR:OG1	1:A:3601:VAL:HG12	2.18	0.43
1:A:3752:VAL:HG12	1:A:3802:LEU:HD13	2.01	0.43
3:C:42:VAL:HG21	3:C:90:LEU:HD11	2.00	0.43
3:C:206:GLU:O	3:C:210:MET:HG2	2.18	0.43
3:C:536:LEU:HD22	3:C:537:PHE:CE1	2.52	0.43
1:A:303:HIS:C	1:A:309:LYS:HZ1	2.26	0.43
1:A:958:MET:N	1:A:958:MET:HE2	2.33	0.43
1:A:1688:LEU:HA	1:A:1691:GLN:HB2	2.00	0.43
1:A:2412:TYR:CE1	1:A:2454:LEU:HD11	2.54	0.43
1:A:2501:LEU:HD12	1:A:2501:LEU:HA	1.81	0.43
1:A:3960:PRO:HD3	1:A:4110:GLN:NE2	2.33	0.43
3:C:65:ASP:H	3:C:78:THR:HG22	1.84	0.43
3:C:194:LEU:H	3:C:194:LEU:HD23	1.84	0.43
3:C:256:ASN:OD1	3:C:256:ASN:N	2.51	0.43
3:C:348:SER:O	3:C:351:VAL:HG12	2.18	0.43
3:C:531:SER:O	3:C:534:LYS:HG2	2.18	0.43
1:A:584:GLU:N	1:A:613:HIS:O	2.42	0.43
1:A:847:SER:O	1:A:851:ILE:HG12	2.18	0.43
1:A:993:HIS:CE1	1:A:1039:TRP:CE2	3.07	0.43
1:A:1148:ALA:HA	1:A:1151:ARG:NH2	2.34	0.43
1:A:1444:ASP:OD1	1:A:1445:ARG:N	2.51	0.43
1:A:1867:ILE:HD11	1:A:1940:TYR:CG	2.54	0.43
1:A:3049:LEU:HD12	1:A:3049:LEU:HA	1.78	0.43
1:A:3988:LEU:HA	1:A:3988:LEU:HD12	1.66	0.43
1:A:4013:TRP:CD1	1:A:4014:LYS:HD3	2.54	0.43
2:B:340:PHE:HD2	2:B:408:PRO:HD2	1.83	0.43
2:B:419:GLU:OE2	2:B:427:VAL:HG22	2.19	0.43
3:C:211:VAL:O	3:C:214:SER:OG	2.33	0.43
3:C:528:ILE:O	3:C:531:SER:OG	2.28	0.43
4:D:31:DA:C6	4:D:32:DA:N6	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:O	1:A:245:SER:CB	2.67	0.42
1:A:410:MET:HE2	1:A:410:MET:HA	2.00	0.42
1:A:2259:LYS:HD2	1:A:2259:LYS:HA	1.84	0.42
1:A:2370:SER:O	1:A:2370:SER:OG	2.35	0.42
1:A:3029:LYS:O	1:A:3032:SER:OG	2.21	0.42
1:A:3459:ASN:HB2	1:A:3462:ARG:NH2	2.33	0.42
1:A:3606:ILE:HA	1:A:3609:MET:HB3	2.01	0.42
1:A:3998:LEU:O	1:A:4002:MET:HG2	2.18	0.42
2:B:41:LEU:HA	2:B:41:LEU:HD12	1.64	0.42
2:B:254:ARG:NH1	2:B:255:ALA:O	2.52	0.42
2:B:514:MET:HA	2:B:517:ARG:HB3	2.01	0.42
1:A:108:LYS:HE3	1:A:108:LYS:HB3	1.87	0.42
1:A:669:LEU:HD12	1:A:669:LEU:HA	1.84	0.42
1:A:967:PRO:O	1:A:971:ARG:HG2	2.19	0.42
1:A:1471:GLN:NE2	1:A:1478:SER:HB3	2.34	0.42
1:A:1601:LEU:O	1:A:1604:SER:N	2.52	0.42
1:A:3008:TRP:CH2	1:A:3050:LYS:HG3	2.54	0.42
1:A:3329:LEU:HD23	1:A:3329:LEU:HA	1.81	0.42
1:A:3710:LYS:HZ1	1:A:3713:PRO:HD2	1.84	0.42
2:B:97:VAL:HG13	2:B:99:PHE:CD1	2.54	0.42
2:B:244:ARG:HA	2:B:244:ARG:NE	2.33	0.42
2:B:463:LYS:NZ	3:C:387:LEU:HD21	2.34	0.42
3:C:197:ILE:HD11	3:C:202:LYS:HG2	2.00	0.42
1:A:35:ILE:HA	1:A:38:LEU:HG	2.01	0.42
1:A:579:LEU:HD23	1:A:579:LEU:HA	1.79	0.42
1:A:784:VAL:HG23	1:A:785:MET:SD	2.59	0.42
1:A:2091:HIS:CG	1:A:2094:MET:HE3	2.53	0.42
1:A:2586:PHE:HB3	1:A:2776:ARG:HB3	2.01	0.42
1:A:2591:ILE:HD12	1:A:2592:ASP:H	1.84	0.42
1:A:2970:LYS:O	1:A:2974:GLU:HB2	2.20	0.42
1:A:3355:LYS:O	1:A:3359:ILE:HD12	2.20	0.42
1:A:3607:GLU:H	1:A:3607:GLU:CD	2.27	0.42
1:A:3613:MET:O	1:A:3617:LEU:HB2	2.20	0.42
2:B:43:ASP:HA	2:B:88:TYR:CZ	2.55	0.42
2:B:77:SER:O	2:B:250:GLU:HG3	2.20	0.42
2:B:214:SER:O	2:B:218:ARG:HD3	2.19	0.42
2:B:264:ASN:OD1	2:B:267:ILE:HG12	2.20	0.42
2:B:270:SER:HB2	2:B:373:SER:HB2	2.01	0.42
2:B:507:THR:O	3:C:394:ARG:HD2	2.20	0.42
1:A:74:ASN:H	1:A:117:LYS:HD2	1.85	0.42
1:A:637:LYS:HE3	1:A:638:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:VAL:HA	1:A:1010:LEU:CB	2.49	0.42
1:A:1527:ARG:NH2	1:A:1531:LEU:HD11	2.34	0.42
1:A:1713:VAL:O	1:A:1716:GLN:HG2	2.20	0.42
1:A:1935:GLU:H	1:A:1935:GLU:CD	2.28	0.42
1:A:2842:ARG:O	1:A:2846:THR:HG23	2.19	0.42
1:A:3232:ARG:HH22	1:A:3265:GLU:HG3	1.83	0.42
2:B:368:VAL:HB	2:B:432:PHE:HB2	2.02	0.42
3:C:246:HIS:CE1	3:C:264:TYR:HH	2.37	0.42
1:A:12:LEU:HD11	1:A:44:LEU:HD23	2.02	0.42
1:A:474:VAL:O	1:A:478:CYS:HB2	2.19	0.42
1:A:1082:PHE:HB2	1:A:1107:TYR:OH	2.18	0.42
1:A:1687:HIS:O	1:A:1691:GLN:N	2.44	0.42
1:A:2127:LYS:HA	1:A:2127:LYS:HD2	1.83	0.42
1:A:3097:ASP:N	1:A:3097:ASP:OD1	2.51	0.42
1:A:3416:LEU:HD23	1:A:3449:LYS:HD3	2.02	0.42
2:B:370:PRO:HG3	2:B:382:PHE:HB3	2.01	0.42
3:C:83:LEU:HD12	3:C:83:LEU:HA	1.78	0.42
1:A:1506:SER:O	1:A:1509:GLN:NE2	2.52	0.42
1:A:1618:LEU:O	1:A:1622:ILE:HG12	2.20	0.42
1:A:1754:GLN:HG2	1:A:1785:ILE:HG13	2.02	0.42
1:A:1869:LYS:HE2	1:A:1869:LYS:HB3	1.72	0.42
1:A:2093:CYS:C	1:A:2096:PRO:HD2	2.45	0.42
1:A:2341:LEU:O	1:A:2345:VAL:HG23	2.20	0.42
1:A:3027:LEU:HA	1:A:3031:TRP:CZ3	2.55	0.42
1:A:3582:GLU:O	1:A:3586:LYS:HG2	2.20	0.42
2:B:341:ASP:OD1	2:B:341:ASP:N	2.52	0.42
2:B:353:LEU:HB2	2:B:393:GLU:O	2.19	0.42
2:B:462:MET:HA	2:B:465:ILE:HB	2.02	0.42
2:B:531:PRO:HB2	2:B:533:ASP:O	2.19	0.42
5:E:20:DT:H2"	5:E:21:DA:C5	2.54	0.42
1:A:254:LYS:O	1:A:300:TRP:NE1	2.50	0.42
1:A:478:CYS:O	1:A:482:VAL:HG23	2.20	0.42
1:A:618:LYS:HE2	1:A:618:LYS:HB2	1.94	0.42
1:A:796:LEU:HD23	1:A:796:LEU:HA	1.80	0.42
1:A:861:SER:HA	1:A:3167:ARG:NH2	2.35	0.42
1:A:978:GLN:OE1	1:A:981:ARG:NH2	2.43	0.42
1:A:1267:TYR:CD2	1:A:1290:LEU:HD13	2.55	0.42
1:A:1356:TRP:CE3	1:A:1356:TRP:CA	3.00	0.42
1:A:1586:SER:HA	1:A:1593:VAL:HG21	2.00	0.42
1:A:2180:GLU:HG3	1:A:2181:GLY:N	2.34	0.42
1:A:2208:ASP:OD1	1:A:2209:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2935:GLU:OE2	1:A:2938:VAL:N	2.35	0.42
1:A:3173:MET:HE1	1:A:3783:GLN:HA	2.01	0.42
3:C:56:LEU:HG	3:C:80:HIS:HB3	2.01	0.42
3:C:261:ILE:HG22	3:C:366:ALA:HA	2.01	0.42
3:C:406:GLY:HA3	3:C:421:TYR:CE1	2.52	0.42
1:A:115:TYR:HB2	1:A:130:LEU:HD21	2.02	0.42
1:A:204:LEU:HD23	1:A:224:LEU:HD13	2.01	0.42
1:A:216:LYS:HZ2	3:C:547:GLN:H	1.66	0.42
1:A:261:ASP:OD1	1:A:265:TYR:CD2	2.73	0.42
1:A:461:ILE:O	1:A:464:VAL:HG12	2.19	0.42
1:A:762:TYR:HB3	1:A:765:LEU:HD12	2.01	0.42
1:A:1527:ARG:O	1:A:1531:LEU:N	2.43	0.42
1:A:1538:LEU:N	1:A:1553:PHE:O	2.50	0.42
1:A:1539:SER:HA	1:A:1552:HIS:ND1	2.35	0.42
1:A:1878:ASP:HB2	1:A:1950:SER:CB	2.49	0.42
1:A:2255:LEU:HD23	1:A:2259:LYS:HG2	2.02	0.42
1:A:3090:TYR:HE2	1:A:3102:TYR:HE2	1.67	0.42
1:A:3107:ILE:HD13	1:A:3107:ILE:HA	1.88	0.42
1:A:3588:TRP:CE2	1:A:3613:MET:HB3	2.55	0.42
1:A:3627:ALA:O	1:A:3630:ARG:HB3	2.20	0.42
1:A:4127:TRP:HD1	1:A:4128:MET:HG2	1.82	0.42
3:C:522:VAL:O	3:C:525:LYS:HG2	2.19	0.42
4:D:38:DT:H6	4:D:38:DT:H2'	1.69	0.42
5:E:26:DT:H1'	5:E:27:DT:H5'	2.01	0.42
1:A:287:LEU:O	1:A:290:TYR:HB2	2.20	0.42
1:A:890:LYS:HA	1:A:890:LYS:HD3	1.75	0.42
1:A:1893:GLU:OE1	1:A:1895:LYS:HG2	2.19	0.42
1:A:2242:VAL:HG13	1:A:2283:ASN:ND2	2.34	0.42
1:A:2974:GLU:O	1:A:2978:LYS:HG2	2.20	0.42
1:A:3758:LEU:HD12	1:A:3801:GLY:HA3	2.01	0.42
1:A:3895:GLU:HG2	1:A:3896:ALA:N	2.35	0.42
2:B:290:ARG:NH2	3:C:308:GLU:O	2.53	0.42
2:B:311:LEU:C	2:B:312:LEU:HD12	2.44	0.42
3:C:53:GLU:OE1	3:C:53:GLU:HA	2.20	0.42
3:C:53:GLU:OE1	3:C:85:LEU:HD23	2.19	0.42
3:C:441:SER:OG	3:C:444:TYR:N	2.50	0.42
1:A:70:ARG:HD3	1:A:70:ARG:H	1.85	0.42
1:A:723:ASP:C	1:A:725:LEU:H	2.28	0.42
1:A:935:HIS:O	1:A:938:VAL:HG12	2.19	0.42
1:A:1132:ASP:OD1	1:A:1136:ARG:NH2	2.53	0.42
1:A:1438:GLY:O	1:A:1445:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:GLN:O	1:A:1798:LEU:HG	2.19	0.42
1:A:1816:ARG:O	1:A:1819:PHE:HB2	2.19	0.42
1:A:2245:TRP:C	1:A:2247:ASP:H	2.27	0.42
1:A:3274:VAL:O	1:A:3278:GLN:NE2	2.51	0.42
1:A:3733:ARG:HA	1:A:3733:ARG:HD2	1.84	0.42
1:A:3828:TYR:HE1	1:A:3835:PRO:HG2	1.84	0.42
2:B:259:LEU:HD23	2:B:259:LEU:HA	1.71	0.42
2:B:290:ARG:HG2	3:C:309:ASP:CA	2.50	0.42
3:C:249:CYS:SG	3:C:338:LYS:HD2	2.60	0.42
3:C:472:THR:HG22	3:C:474:GLU:OE1	2.19	0.42
4:D:42:DA:N6	5:E:14:DT:H1'	2.35	0.42
1:A:540:MET:O	1:A:544:ILE:HG12	2.20	0.41
1:A:606:SER:N	1:A:1027:ASP:OD1	2.53	0.41
1:A:800:LEU:HD23	1:A:800:LEU:H	1.85	0.41
1:A:1257:LEU:HD23	1:A:1257:LEU:HA	1.90	0.41
1:A:1482:GLU:HA	1:A:1486:LEU:HD13	2.02	0.41
1:A:2138:VAL:CB	1:A:2139:PRO:CD	2.78	0.41
1:A:2415:LEU:HD12	1:A:2415:LEU:HA	1.72	0.41
1:A:3129:LEU:O	1:A:3132:VAL:HG12	2.20	0.41
2:B:330:GLU:H	2:B:333:GLU:CD	2.22	0.41
3:C:93:ASP:CG	3:C:97:LYS:HB2	2.45	0.41
3:C:185:LEU:HD12	3:C:511:HIS:HD2	1.84	0.41
1:A:57:LEU:HG	1:A:103:TYR:CZ	2.55	0.41
1:A:78:PHE:HA	1:A:81:CYS:SG	2.60	0.41
1:A:239:GLU:H	1:A:243:GLN:NE2	2.13	0.41
1:A:359:LEU:O	1:A:363:ILE:HG12	2.19	0.41
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.83	0.41
1:A:749:VAL:O	1:A:753:GLN:HG3	2.20	0.41
1:A:941:MET:HE3	1:A:941:MET:HB3	1.95	0.41
1:A:1037:LEU:HD12	1:A:1037:LEU:HA	1.85	0.41
1:A:1050:GLU:CD	1:A:1050:GLU:H	2.27	0.41
1:A:1725:GLN:HG3	1:A:1728:GLU:HG2	2.02	0.41
1:A:1773:VAL:H	1:A:1775:GLU:CD	2.23	0.41
1:A:1833:LEU:C	1:A:1835:ALA:H	2.28	0.41
1:A:2947:ILE:HG13	1:A:2948:GLY:N	2.35	0.41
1:A:3355:LYS:HA	1:A:3355:LYS:HD2	1.90	0.41
1:A:3592:VAL:O	1:A:3595:GLU:HG3	2.20	0.41
1:A:3646:LYS:HZ2	1:A:3653:ARG:HH12	1.67	0.41
2:B:115:ARG:O	2:B:119:LEU:HD23	2.19	0.41
2:B:244:ARG:HA	2:B:244:ARG:HE	1.85	0.41
2:B:303:PHE:CD1	2:B:310:LEU:HD13	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:HIS:HB3	3:C:411:HIS:CD2	2.55	0.41
2:B:400:TYR:CE2	2:B:402:PRO:HG3	2.55	0.41
2:B:421:ASP:HB2	2:B:425:ILE:HB	2.02	0.41
3:C:271:ARG:O	3:C:273:LYS:NZ	2.52	0.41
3:C:377:LEU:O	3:C:381:ILE:HG12	2.20	0.41
1:A:288:ASP:OD1	1:A:288:ASP:N	2.50	0.41
1:A:372:PRO:O	1:A:375:VAL:HG22	2.18	0.41
1:A:450:SER:OG	1:A:453:MET:HG3	2.21	0.41
1:A:1503:LEU:HB2	1:A:1508:LYS:HE2	2.01	0.41
1:A:2098:THR:O	1:A:2102:LYS:HG2	2.20	0.41
1:A:3080:LEU:HD23	1:A:3081:HIS:CE1	2.55	0.41
1:A:3195:GLU:OE1	1:A:3195:GLU:N	2.47	0.41
1:A:3307:LEU:C	1:A:3309:GLU:H	2.28	0.41
1:A:3974:MET:N	1:A:3974:MET:SD	2.94	0.41
2:B:90:THR:OG1	2:B:91:GLU:N	2.52	0.41
2:B:497:LEU:HD12	2:B:500:PRO:HG3	2.01	0.41
4:D:33:DA:H2"	4:D:34:DC:C6	2.55	0.41
1:A:26:GLY:HA3	1:A:29:LEU:HD21	2.01	0.41
1:A:407:VAL:O	1:A:410:MET:HB2	2.19	0.41
1:A:892:LEU:HA	1:A:892:LEU:HD23	1.75	0.41
1:A:1214:GLU:HG2	1:A:1215:GLU:OE1	2.21	0.41
1:A:1282:LEU:HD23	1:A:1282:LEU:H	1.86	0.41
1:A:2150:VAL:HG13	1:A:2157:PHE:CE2	2.55	0.41
1:A:3044:MET:HE2	1:A:3044:MET:HB2	1.90	0.41
1:A:3098:ARG:HD2	1:A:3098:ARG:HA	1.90	0.41
1:A:3452:LYS:HE2	1:A:3452:LYS:HB2	1.84	0.41
1:A:350:ARG:NH1	1:A:351:ASN:HB2	2.35	0.41
1:A:1098:GLN:HG3	1:A:1152:ARG:HG3	2.02	0.41
1:A:1198:LEU:HB3	1:A:1199:PRO:HD2	2.02	0.41
1:A:1207:TRP:O	1:A:1211:VAL:HG13	2.21	0.41
1:A:1576:ASP:O	1:A:1580:LEU:HG	2.20	0.41
1:A:1867:ILE:O	1:A:1871:MET:HG3	2.20	0.41
1:A:1898:GLN:OE1	1:A:1898:GLN:N	2.54	0.41
1:A:1923:PHE:HA	1:A:1941:HIS:HD2	1.86	0.41
1:A:2270:ASN:O	1:A:2274:ILE:HG13	2.21	0.41
1:A:2332:GLU:HB3	1:A:2335:ASN:C	2.45	0.41
1:A:2353:GLN:HA	1:A:2356:MET:O	2.20	0.41
1:A:2398:LEU:HA	1:A:2398:LEU:HD23	1.84	0.41
1:A:2563:LEU:HD23	1:A:2563:LEU:HA	1.73	0.41
1:A:3255:ALA:CB	1:A:3283:LEU:HD11	2.48	0.41
1:A:3259:LEU:HD12	1:A:3259:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3358:ARG:NH2	1:A:3361:GLU:OE2	2.48	0.41
1:A:3466:PRO:HB2	1:A:4004:VAL:HG11	2.02	0.41
1:A:3562:LEU:O	1:A:3564:GLN:NE2	2.53	0.41
2:B:243:LEU:O	2:B:245:LYS:N	2.53	0.41
3:C:40:MET:HA	3:C:43:GLN:CG	2.50	0.41
3:C:156:LYS:HD2	3:C:156:LYS:HA	1.80	0.41
3:C:339:CYS:SG	3:C:340:PHE:N	2.94	0.41
1:A:333:MET:SD	1:A:334:HIS:CE1	3.14	0.41
1:A:944:LYS:HD3	1:A:944:LYS:HA	1.87	0.41
1:A:1119:LYS:HA	1:A:1119:LYS:HD3	1.91	0.41
1:A:1186:LYS:HD3	1:A:1186:LYS:HA	1.90	0.41
1:A:1649:LEU:HA	1:A:1652:ILE:HG22	2.01	0.41
1:A:1905:ILE:HG23	1:A:1905:ILE:O	2.20	0.41
1:A:2820:MET:HA	1:A:2823:PHE:CE1	2.55	0.41
1:A:3232:ARG:NH2	1:A:3265:GLU:HG3	2.35	0.41
1:A:3767:LEU:HA	1:A:3767:LEU:HD23	1.73	0.41
1:A:3809:THR:HG22	1:A:3931:ALA:HA	2.02	0.41
1:A:4070:LYS:HA	1:A:4070:LYS:HD3	1.82	0.41
2:B:83:LEU:HD23	2:B:83:LEU:HA	1.95	0.41
2:B:106:GLN:HG2	2:B:115:ARG:NE	2.36	0.41
2:B:140:ASP:N	2:B:140:ASP:OD1	2.49	0.41
2:B:349:GLY:HA3	3:C:463:LEU:CD2	2.50	0.41
3:C:314:PHE:O	3:C:320:ILE:HA	2.20	0.41
3:C:412:ILE:HD12	3:C:417:GLU:CD	2.46	0.41
1:A:19:LEU:HD12	1:A:34:LEU:HA	2.01	0.41
1:A:215:PRO:HB2	1:A:216:LYS:HD3	2.02	0.41
1:A:1111:LEU:HD12	1:A:1111:LEU:HA	1.90	0.41
1:A:1483:LEU:HD22	1:A:1524:LEU:HD21	2.03	0.41
1:A:1759:LEU:O	1:A:1763:THR:HG23	2.20	0.41
1:A:2227:LYS:HA	1:A:2227:LYS:HD2	1.75	0.41
1:A:2321:GLU:O	1:A:2325:LEU:HD23	2.20	0.41
1:A:3074:GLN:O	1:A:3078:LEU:HB3	2.20	0.41
1:A:3357:ARG:HG2	1:A:3358:ARG:HG2	2.03	0.41
1:A:3662:ILE:O	1:A:3665:MET:HG3	2.20	0.41
1:A:4061:CYS:SG	1:A:4062:ASP:N	2.94	0.41
2:B:464:ALA:O	2:B:467:GLU:HG3	2.20	0.41
3:C:402:ASN:OD1	3:C:402:ASN:N	2.54	0.41
5:E:18:DA:OP2	5:E:18:DA:H2'	2.20	0.41
1:A:278:HIS:CD2	1:A:281:GLN:HG3	2.52	0.41
1:A:390:GLN:HA	1:A:393:LYS:NZ	2.36	0.41
1:A:990:GLN:HB3	1:A:2781:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1629:CYS:O	1:A:1633:TRP:NE1	2.50	0.41
1:A:1678:LEU:HD23	1:A:1678:LEU:HA	1.91	0.41
1:A:1938:ARG:NH1	1:A:1975:LEU:O	2.53	0.41
1:A:3133:GLN:HE21	1:A:3167:ARG:HD3	1.84	0.41
2:B:213:ILE:HG22	2:B:214:SER:H	1.85	0.41
3:C:10:VAL:HG22	3:C:53:GLU:O	2.21	0.41
3:C:88:PHE:HD1	3:C:91:LEU:HD21	1.85	0.41
3:C:205:LEU:HA	3:C:208:VAL:HG22	2.02	0.41
3:C:274:LYS:HA	3:C:274:LYS:HE2	2.02	0.41
3:C:376:ALA:O	3:C:380:LEU:HG	2.21	0.41
1:A:71:LYS:HB2	1:A:73:LEU:HG	2.03	0.41
1:A:120:ALA:HB1	1:A:127:ALA:HA	2.02	0.41
1:A:148:LYS:O	1:A:152:LEU:HG	2.21	0.41
1:A:394:GLN:HG2	1:A:1687:HIS:HB2	2.02	0.41
1:A:919:LEU:HA	1:A:919:LEU:HD23	1.82	0.41
1:A:1336:THR:HA	1:A:1339:VAL:HG22	2.03	0.41
1:A:1503:LEU:HB2	1:A:1508:LYS:CE	2.51	0.41
1:A:1582:LEU:HA	1:A:1582:LEU:HD23	1.78	0.41
1:A:1808:ASP:OD1	1:A:1808:ASP:N	2.50	0.41
1:A:1812:LEU:HG	1:A:1814:PHE:H	1.86	0.41
1:A:2088:LEU:HA	1:A:2094:MET:HG3	2.02	0.41
1:A:2126:MET:HE2	1:A:2126:MET:HB3	1.95	0.41
1:A:2150:VAL:HG13	1:A:2157:PHE:CD2	2.56	0.41
1:A:2187:VAL:HG23	1:A:2188:GLU:HG2	2.02	0.41
1:A:2217:ASN:HA	1:A:2220:MET:HG2	2.03	0.41
1:A:2549:LYS:HE2	1:A:2549:LYS:HB2	1.93	0.41
1:A:3020:ASP:CG	1:A:3023:ASN:HD21	2.29	0.41
1:A:3110:PHE:CD1	1:A:3110:PHE:C	2.99	0.41
1:A:3157:LEU:O	1:A:3161:LEU:HG	2.20	0.41
1:A:3586:LYS:O	1:A:3589:SER:OG	2.33	0.41
1:A:3611:GLU:OE2	1:A:3612:ARG:HG2	2.21	0.41
1:A:3828:TYR:CZ	1:A:4128:MET:HE3	2.56	0.41
1:A:3828:TYR:CE1	1:A:3835:PRO:HG2	2.56	0.41
2:B:46:LYS:HA	2:B:49:PHE:HD1	1.85	0.41
2:B:456:PRO:O	2:B:459:VAL:HG22	2.21	0.41
3:C:365:PHE:CZ	3:C:416:TYR:HE2	2.38	0.41
3:C:431:ARG:HD3	3:C:431:ARG:HA	1.96	0.41
3:C:442:LYS:HA	3:C:442:LYS:HD3	1.98	0.41
4:D:41:DT:H2"	4:D:42:DA:C8	2.55	0.41
1:A:87:LYS:NZ	1:A:91:ILE:HD11	2.35	0.41
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASN:N	1:A:336:ASN:OD1	2.53	0.41
1:A:922:SER:C	1:A:924:ARG:H	2.29	0.41
1:A:993:HIS:ND1	1:A:1039:TRP:CD2	2.89	0.41
1:A:1086:TYR:CG	1:A:1087:ARG:N	2.89	0.41
1:A:1166:LEU:O	1:A:1170:LYS:NZ	2.54	0.41
1:A:1722:PHE:HZ	1:A:1742:CYS:SG	2.44	0.41
1:A:1851:LEU:HA	1:A:1851:LEU:HD23	1.85	0.41
1:A:1933:LEU:HB2	1:A:1936:ARG:HB2	2.02	0.41
1:A:1977:ILE:HD12	1:A:1977:ILE:HA	1.95	0.41
1:A:2466:SER:O	1:A:2467:THR:OG1	2.31	0.41
1:A:2563:LEU:C	1:A:2565:MET:N	2.78	0.41
1:A:2957:LEU:HD23	1:A:2957:LEU:HA	1.82	0.41
1:A:2959:ALA:HA	1:A:2962:ARG:NH2	2.36	0.41
1:A:3334:TYR:HB3	1:A:3381:ALA:HB2	2.03	0.41
1:A:3610:TYR:O	1:A:3614:TYR:HD2	2.04	0.41
1:A:3743:HIS:C	1:A:3745:GLU:H	2.29	0.41
3:C:482:ILE:HG22	3:C:483:PRO:O	2.20	0.41
4:D:24:DA:C2	4:D:25:DA:C4	3.09	0.41
1:A:245:SER:O	1:A:248:ILE:HG12	2.22	0.40
1:A:786:GLN:HB3	1:A:787:PRO:HD3	2.03	0.40
1:A:1066:LEU:HD23	1:A:1066:LEU:HA	1.84	0.40
1:A:1195:VAL:N	1:A:1196:PRO:HD2	2.36	0.40
1:A:1651:LYS:HB3	1:A:1651:LYS:HE3	1.82	0.40
1:A:1860:GLU:HG2	1:A:1863:PHE:H	1.86	0.40
1:A:2178:GLY:O	1:A:2183:HIS:NE2	2.54	0.40
1:A:2371:PHE:CD2	1:A:2374:LEU:HG	2.56	0.40
1:A:2923:TRP:CH2	1:A:2946:GLU:HG3	2.56	0.40
1:A:3067:LYS:C	1:A:3070:HIS:HD1	2.27	0.40
1:A:3413:TYR:OH	1:A:3452:LYS:HG2	2.20	0.40
1:A:3517:SER:HA	1:A:3520:GLU:OE1	2.20	0.40
1:A:3742:GLY:C	1:A:3744:ASP:N	2.79	0.40
1:A:3810:VAL:HB	1:A:3932:MET:HE2	2.01	0.40
2:B:66:CYS:O	2:B:70:VAL:HG23	2.21	0.40
2:B:274:TYR:O	2:B:367:PHE:N	2.54	0.40
2:B:404:ARG:NE	2:B:404:ARG:HA	2.35	0.40
3:C:107:PHE:O	3:C:111:LEU:HG	2.21	0.40
1:A:759:GLY:HA3	1:A:766:ALA:HB2	2.03	0.40
1:A:1146:ASN:C	1:A:1146:ASN:HD22	2.28	0.40
1:A:1202:ARG:HB3	1:A:1207:TRP:HB2	2.02	0.40
1:A:1245:ARG:HE	1:A:1246:GLY:N	2.20	0.40
1:A:1443:VAL:HG23	1:A:1447:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:SER:C	1:A:1503:LEU:HD23	2.46	0.40
1:A:1617:LYS:O	1:A:1621:THR:HG23	2.20	0.40
1:A:2231:PHE:CZ	1:A:2235:LEU:HD11	2.57	0.40
1:A:2557:LEU:HD13	1:A:2557:LEU:HA	1.86	0.40
1:A:3330:LEU:HD12	1:A:3330:LEU:HA	1.91	0.40
1:A:3379:GLN:O	1:A:3383:GLN:HG3	2.21	0.40
1:A:3971:MET:O	1:A:3971:MET:HG2	2.20	0.40
2:B:57:LEU:HB3	2:B:62:MET:HG3	2.02	0.40
2:B:389:CYS:HA	2:B:392:LYS:CB	2.47	0.40
3:C:261:ILE:HB	3:C:365:PHE:O	2.21	0.40
1:A:450:SER:O	1:A:454:GLN:HG3	2.22	0.40
1:A:1473:THR:HG22	1:A:1474:ASP:N	2.37	0.40
1:A:1524:LEU:HD12	1:A:1524:LEU:HA	1.87	0.40
1:A:1710:LEU:HA	1:A:1713:VAL:CG2	2.47	0.40
1:A:1736:PHE:O	1:A:1740:VAL:HG13	2.21	0.40
1:A:1933:LEU:HD21	1:A:1937:ARG:NH1	2.32	0.40
1:A:2168:LEU:HD12	1:A:2168:LEU:HA	1.83	0.40
1:A:2383:PHE:HB3	1:A:2418:LYS:NZ	2.37	0.40
1:A:2891:ARG:HD2	1:A:2891:ARG:HA	1.82	0.40
1:A:2897:LEU:HD23	1:A:2897:LEU:HA	1.89	0.40
1:A:2948:GLY:HA2	1:A:2990:GLU:CD	2.47	0.40
1:A:3102:TYR:HA	1:A:3105:ASN:HD22	1.86	0.40
1:A:3312:VAL:HG22	1:A:3315:TYR:CZ	2.56	0.40
2:B:125:GLN:C	2:B:129:LYS:HZ2	2.30	0.40
2:B:378:SER:C	2:B:380:THR:N	2.80	0.40
2:B:454:ALA:HB2	3:C:375:VAL:O	2.21	0.40
3:C:148:ASP:O	3:C:151:ILE:HG22	2.21	0.40
3:C:212:MET:HE1	3:C:220:GLY:O	2.21	0.40
1:A:555:SER:HB3	1:A:1549:SER:HA	2.04	0.40
1:A:1180:GLN:H	1:A:1180:GLN:CD	2.29	0.40
1:A:1209:LYS:NZ	1:A:1210:ASP:OD1	2.53	0.40
1:A:1337:VAL:HG12	1:A:1341:ILE:HD11	2.02	0.40
1:A:1562:LEU:HD23	1:A:1562:LEU:HA	1.85	0.40
1:A:2140:LEU:O	1:A:2144:LEU:HD12	2.21	0.40
1:A:2558:ALA:O	1:A:2562:LEU:HD23	2.21	0.40
1:A:2791:ILE:HD13	1:A:2791:ILE:HA	1.87	0.40
2:B:73:SER:HB2	2:B:244:ARG:HH22	1.86	0.40
2:B:331:LYS:O	2:B:335:GLU:HG3	2.22	0.40
3:C:93:ASP:O	3:C:98:ILE:HG12	2.21	0.40
3:C:513:TRP:O	3:C:516:LEU:N	2.54	0.40
1:A:13:LEU:HA	1:A:59:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ASP:C	1:A:925:GLN:N	2.79	0.40
1:A:2571:ASP:N	1:A:2571:ASP:OD1	2.53	0.40
1:A:3268:THR:HG22	1:A:3269:ARG:HG3	2.03	0.40
1:A:3614:TYR:CD1	1:A:3640:PHE:HZ	2.40	0.40
1:A:4108:MET:O	1:A:4112:THR:HG22	2.21	0.40
2:B:48:MET:O	2:B:59:PRO:HD2	2.22	0.40
2:B:473:TYR:O	2:B:473:TYR:CG	2.74	0.40
2:B:474:ARG:HB3	2:B:476:ASP:OD1	2.21	0.40
3:C:185:LEU:CD2	3:C:514:ASN:HB3	2.52	0.40
3:C:202:LYS:O	3:C:205:LEU:HG	2.20	0.40
3:C:423:GLN:HG2	3:C:424:LEU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3649/4156 (88%)	3291 (90%)	351 (10%)	7 (0%)	43	75
2	B	485/609 (80%)	431 (89%)	53 (11%)	1 (0%)	43	75
3	C	535/732 (73%)	491 (92%)	44 (8%)	0	100	100
All	All	4669/5497 (85%)	4213 (90%)	448 (10%)	8 (0%)	44	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	SER
1	A	2330	VAL
2	B	385	LEU
1	A	1390	GLN
1	A	2134	GLY
1	A	2352	HIS

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Mol	Chain	Res	Type
1	A	2136	PRO
1	A	2331	MET

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3153/3671 (86%)	3149 (100%)	4 (0%)	88	89
2	B	433/548 (79%)	433 (100%)	0	100	100
3	C	466/649 (72%)	466 (100%)	0	100	100
All	All	4052/4868 (83%)	4048 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	SER
1	A	1356	TRP
1	A	1404	LYS
1	A	3483	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	109	ASN
1	A	192	ASN
1	A	243	GLN
1	A	325	ASN
1	A	334	HIS
1	A	442	GLN
1	A	720	GLN
1	A	1043	GLN
1	A	1320	ASN
1	A	1394	HIS

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Mol	Chain	Res	Type
1	A	2365	ASN
1	A	2787	HIS
1	A	2807	GLN
1	A	2845	ASN
1	A	2859	GLN
1	A	3004	HIS
1	A	3023	ASN
1	A	3081	HIS
1	A	3093	GLN
1	A	3105	ASN
1	A	3133	GLN
1	A	3564	GLN
1	A	3743	HIS
1	A	3927	ASN
1	A	3966	GLN
2	B	110	ASN
2	B	293	ASN
2	B	360	HIS
3	C	76	ASN
3	C	547	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	93.14
1	A	5016:UNK	C	6004:UNK	N	49.17

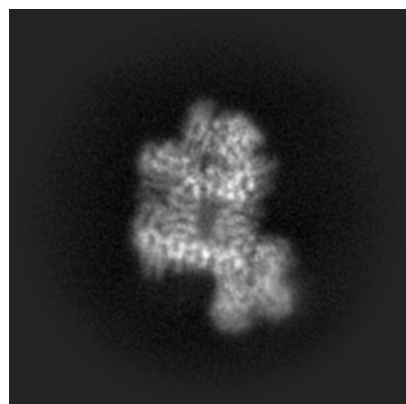
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11217. These allow visual inspection of the internal detail of the map and identification of artifacts.

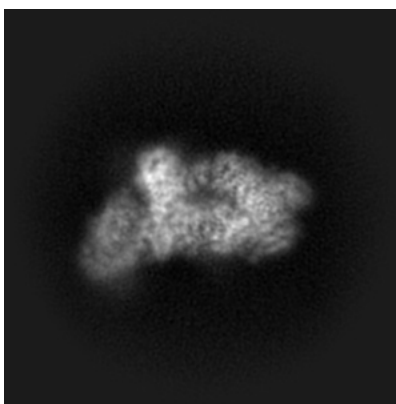
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

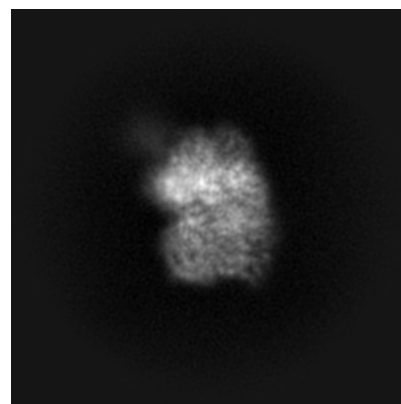
6.1.1 Primary map



X

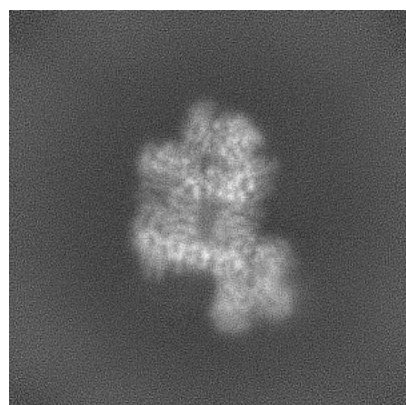


Y

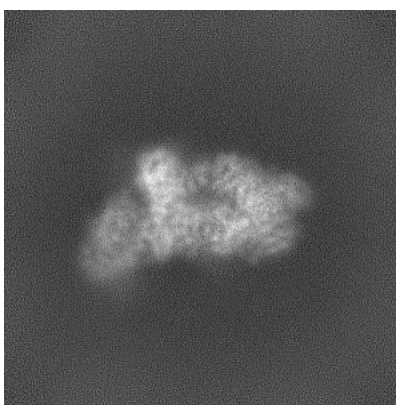


Z

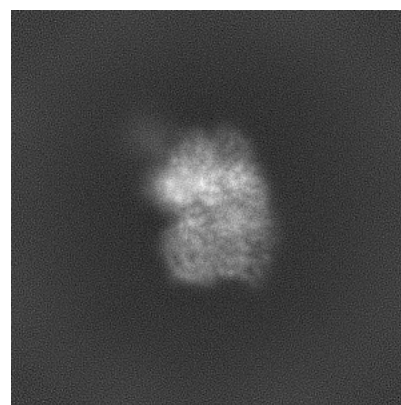
6.1.2 Raw map



X



Y

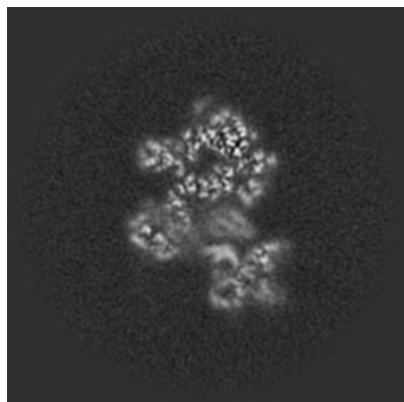


Z

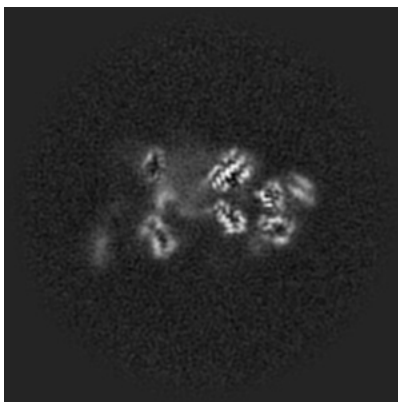
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

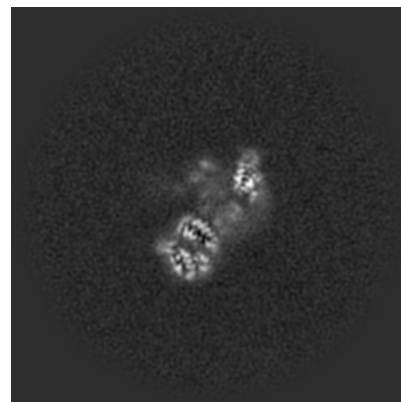
6.2.1 Primary map



X Index: 170

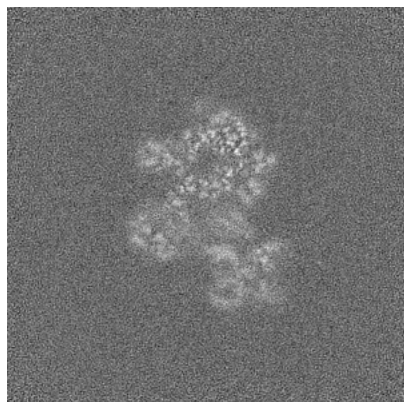


Y Index: 170

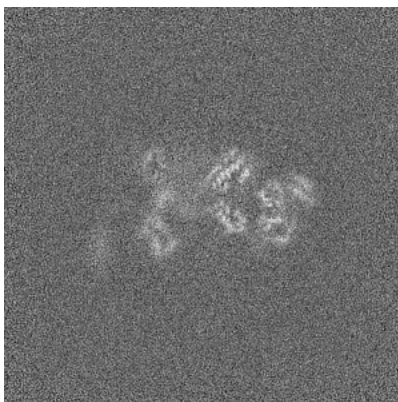


Z Index: 170

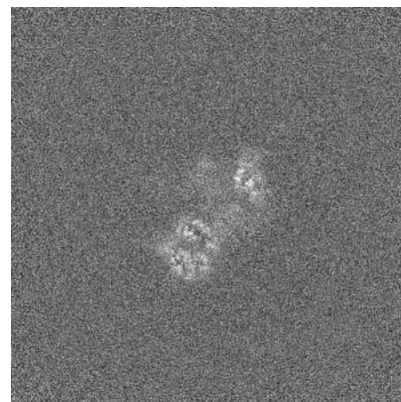
6.2.2 Raw map



X Index: 170



Y Index: 170

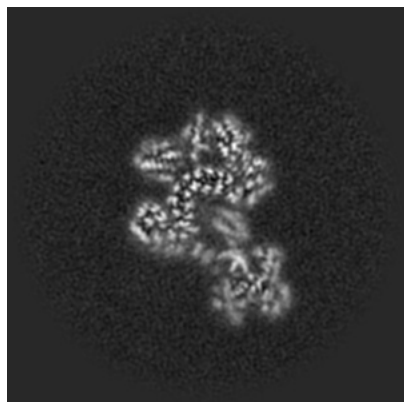


Z Index: 170

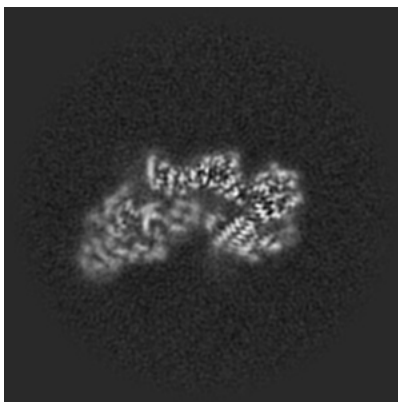
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

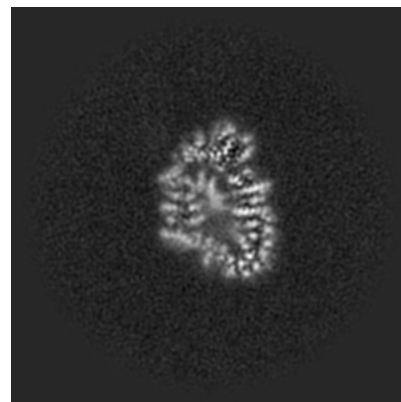
6.3.1 Primary map



X Index: 161

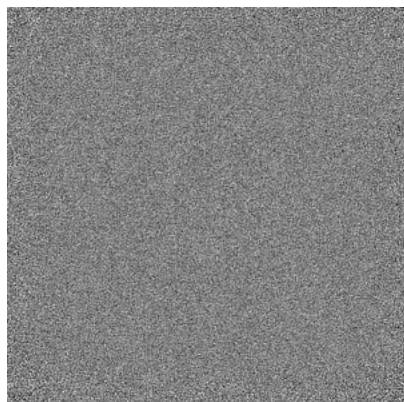


Y Index: 194

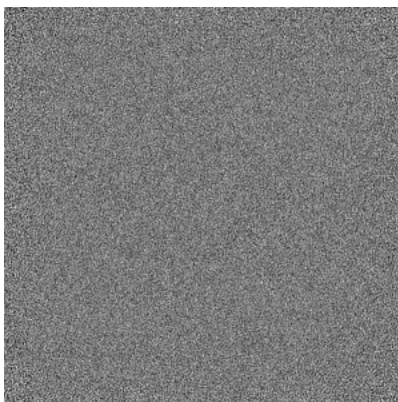


Z Index: 131

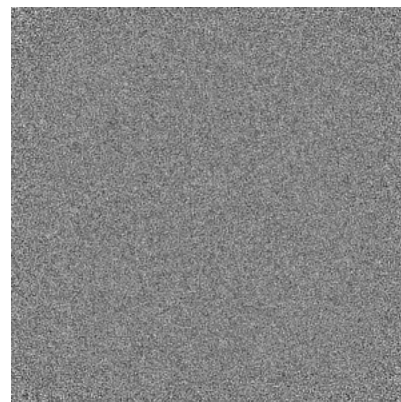
6.3.2 Raw map



X Index: 0



Y Index: 0

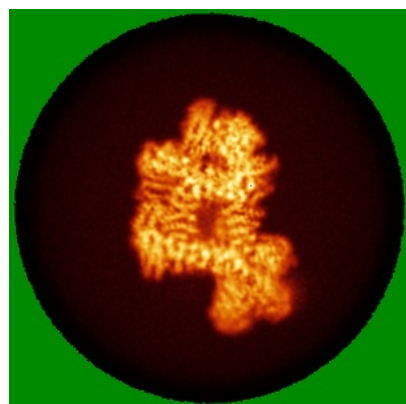


Z Index: 0

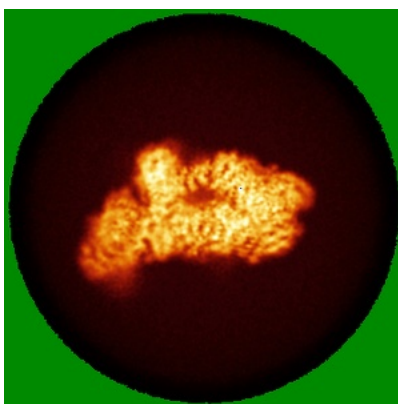
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

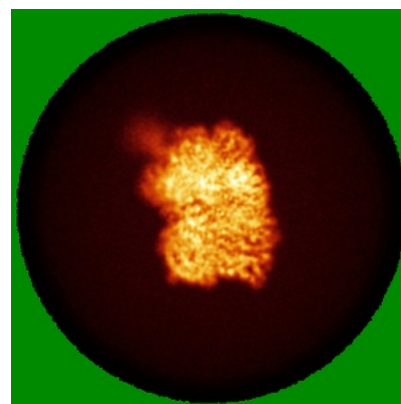
6.4.1 Primary map



X

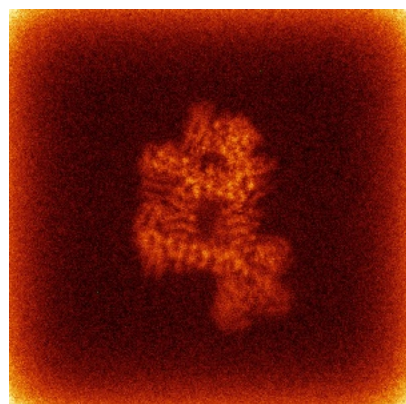


Y

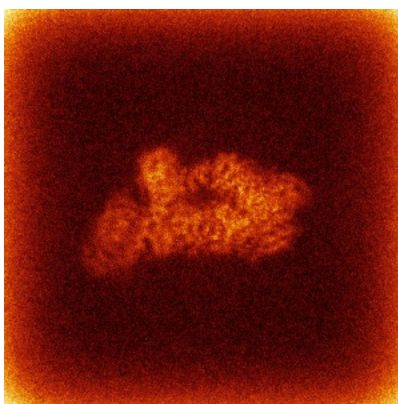


Z

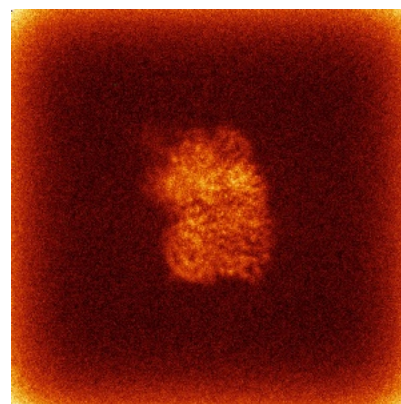
6.4.2 Raw map



X



Y

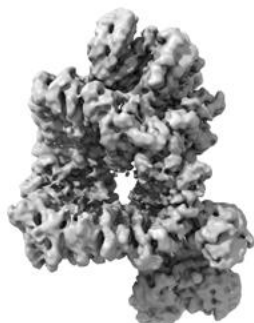


Z

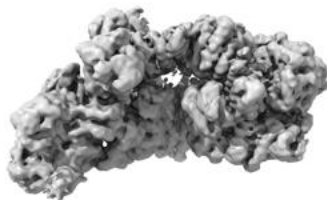
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



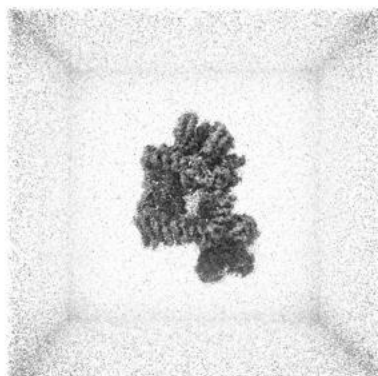
Y



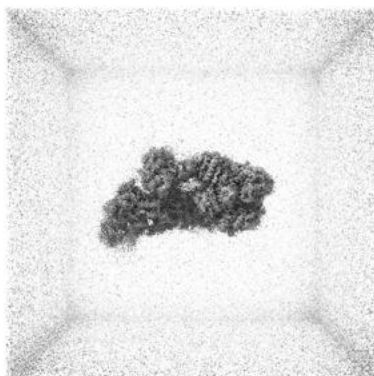
Z

The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

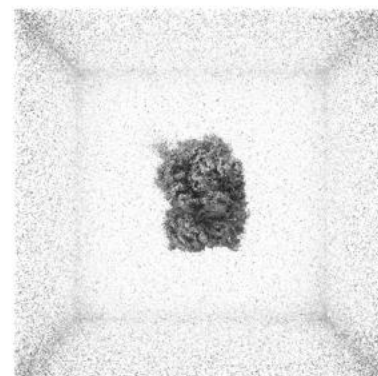
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

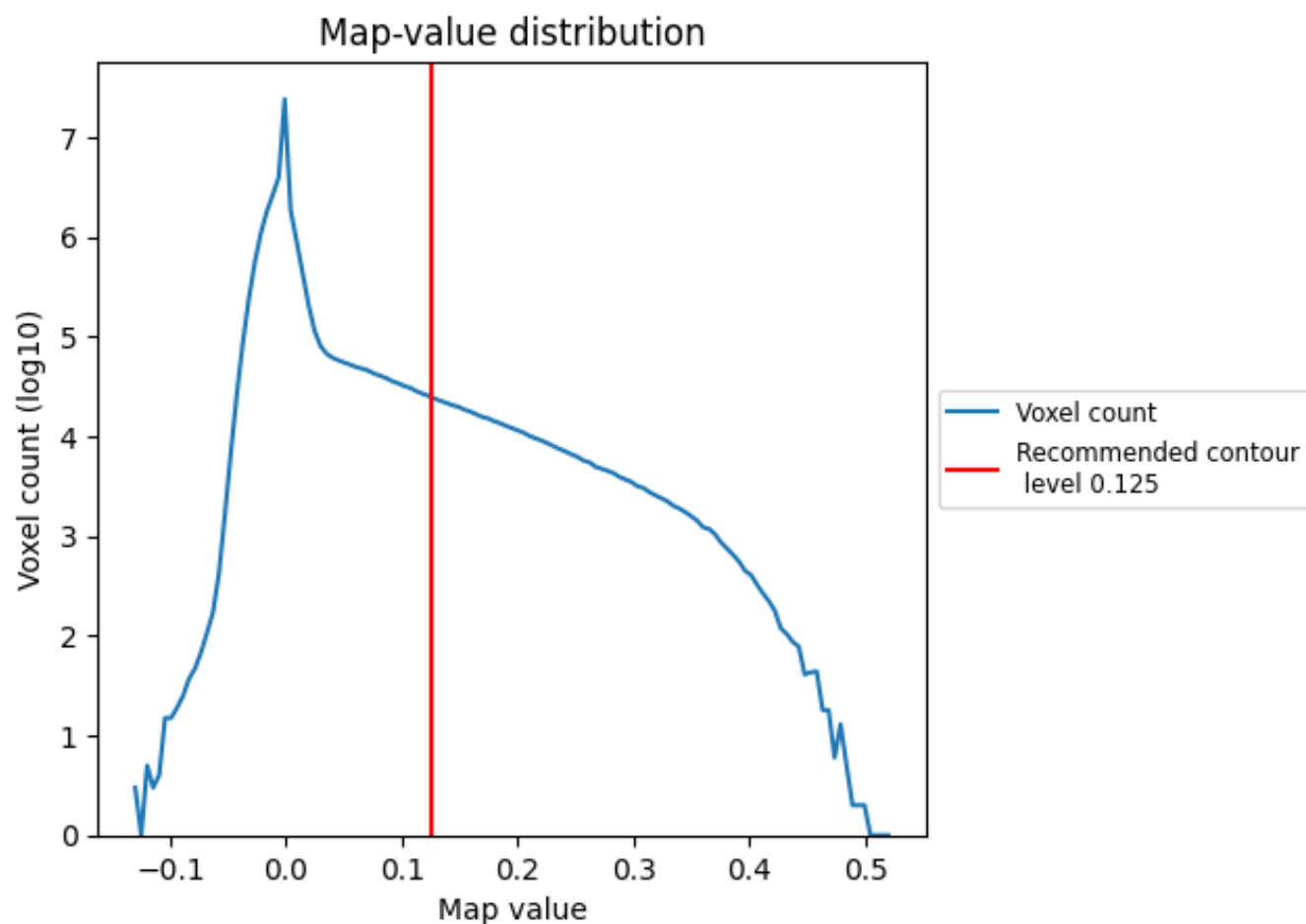
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

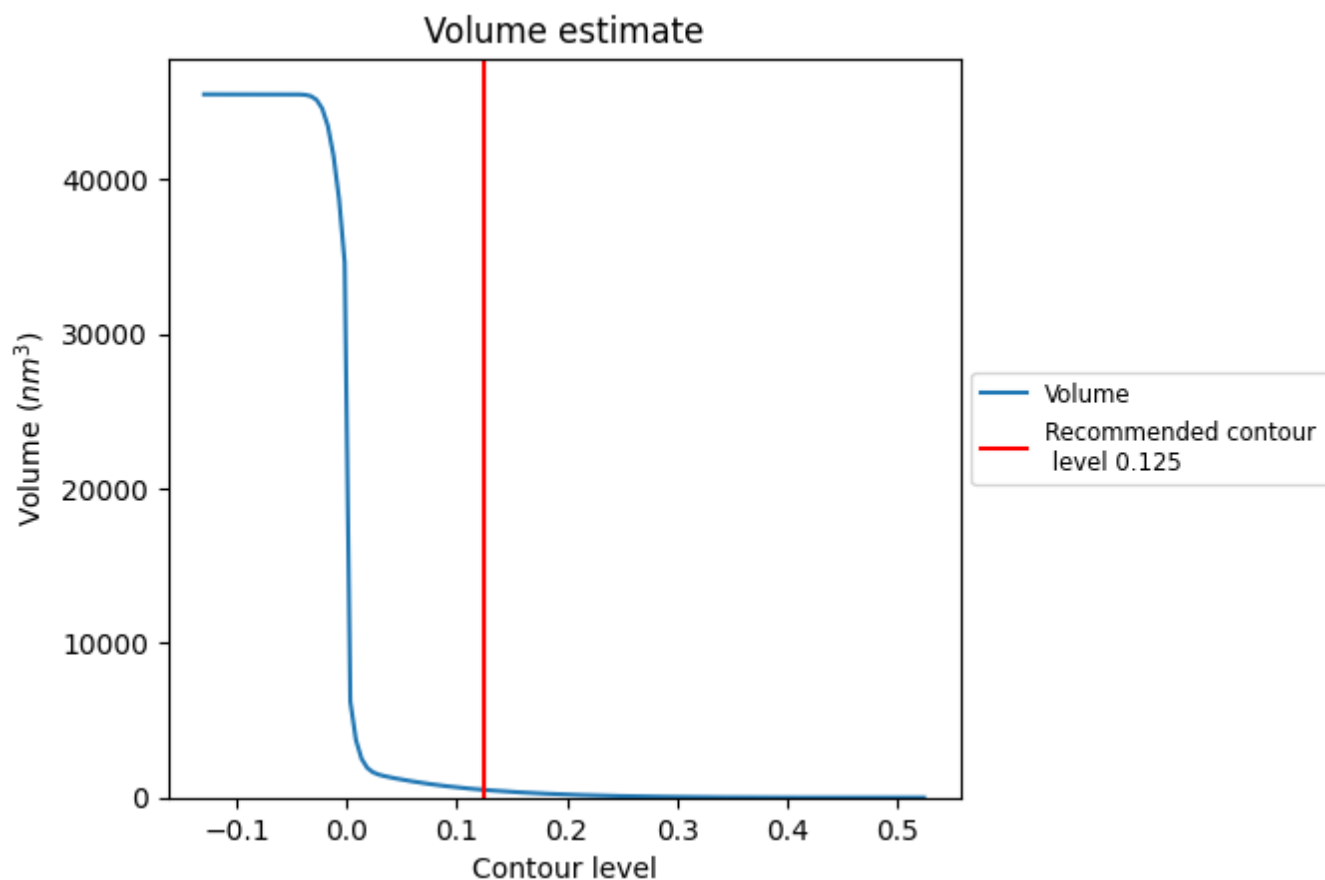
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

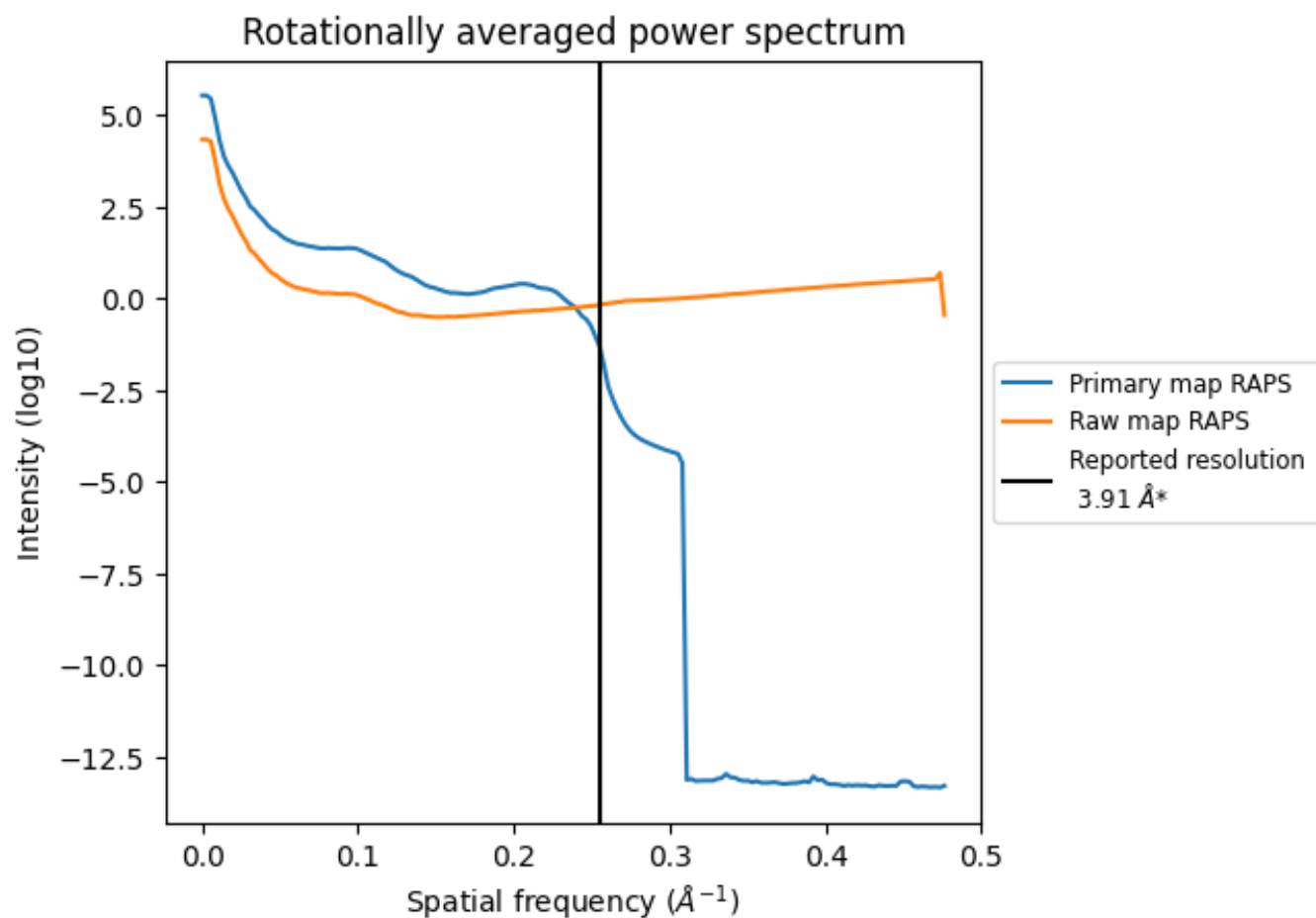
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

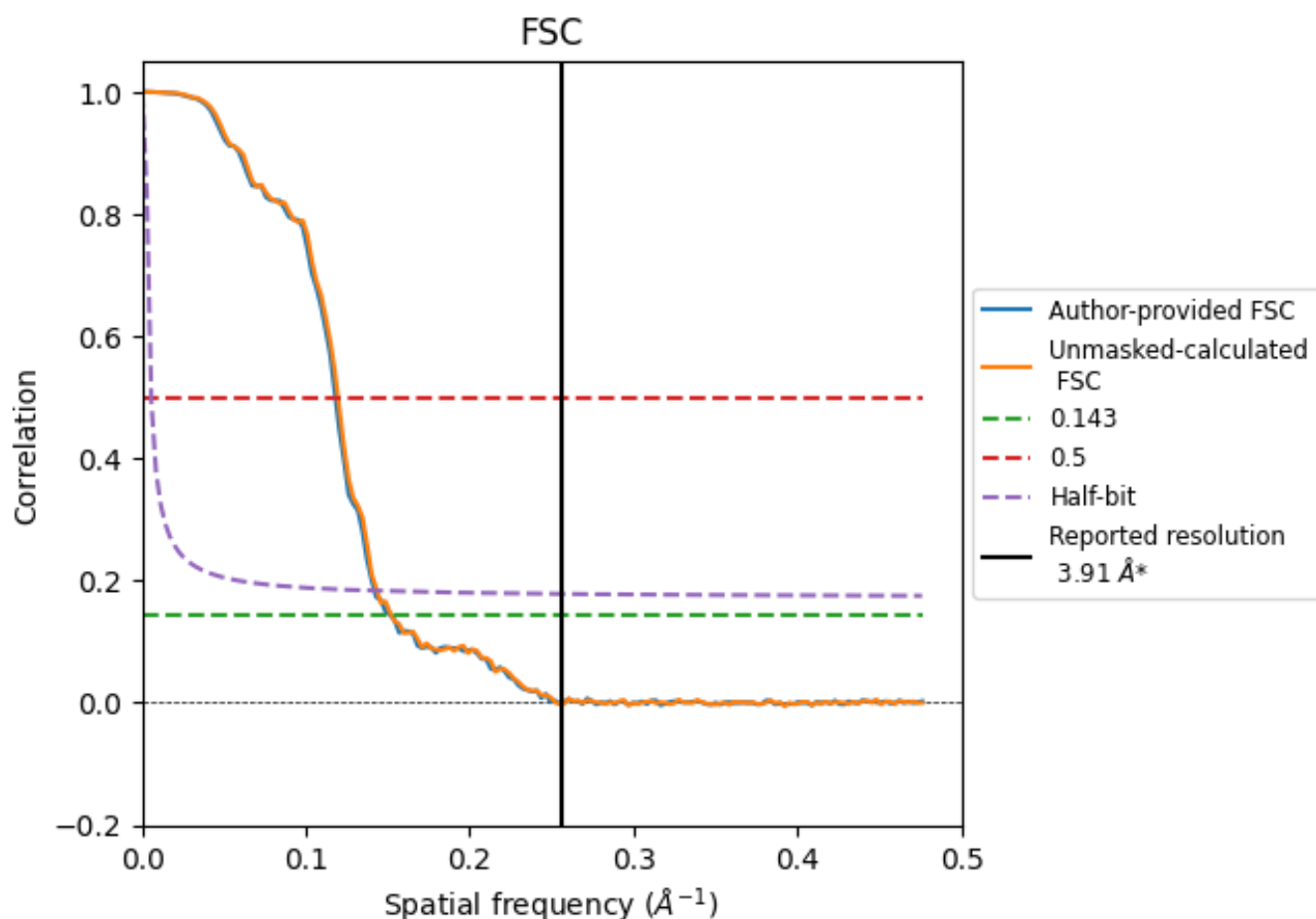


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	6.60	8.47	7.05
Unmasked-calculated*	6.57	8.37	6.98

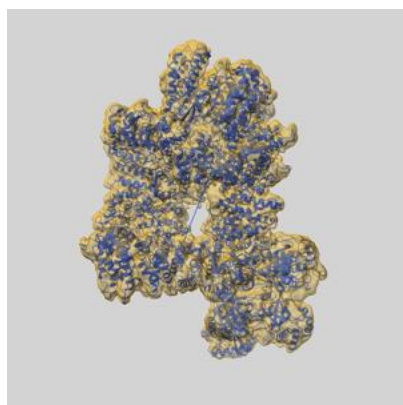
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.60 differs from the reported value 3.91 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.57 differs from the reported value 3.91 by more than 10 %

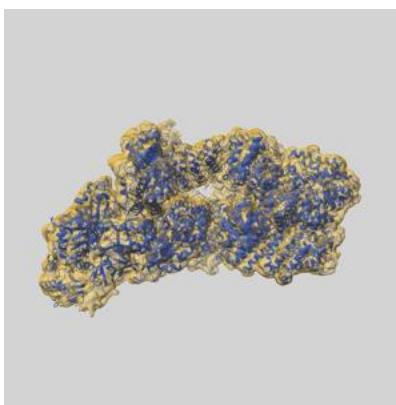
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11217 and PDB model 6ZHA. Per-residue inclusion information can be found in section 3 on page 5.

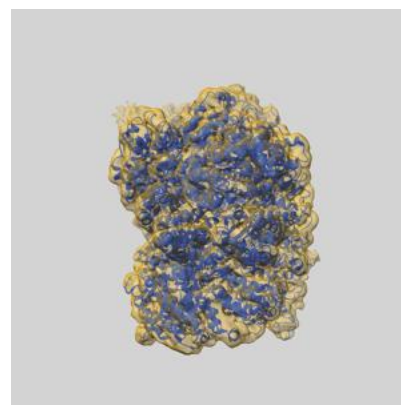
9.1 Map-model overlay [i](#)



X



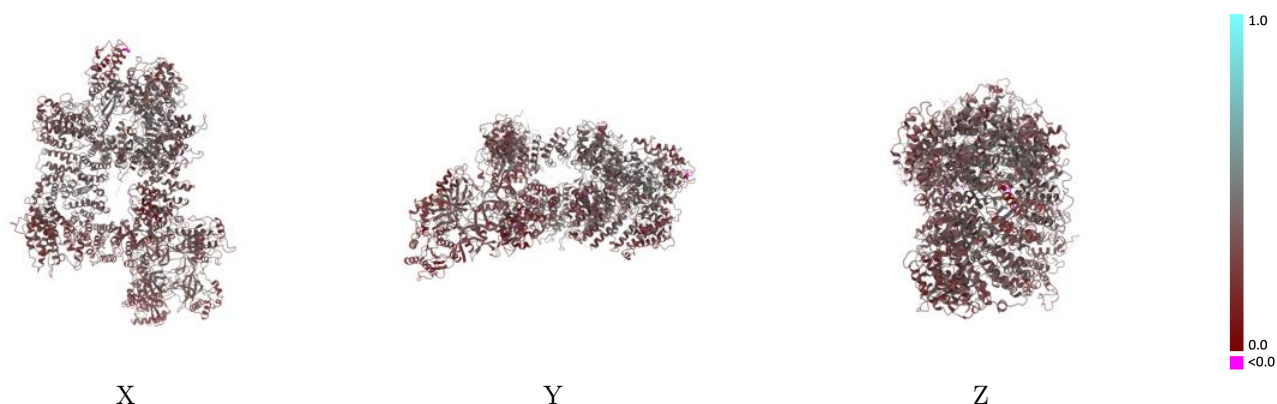
Y



Z

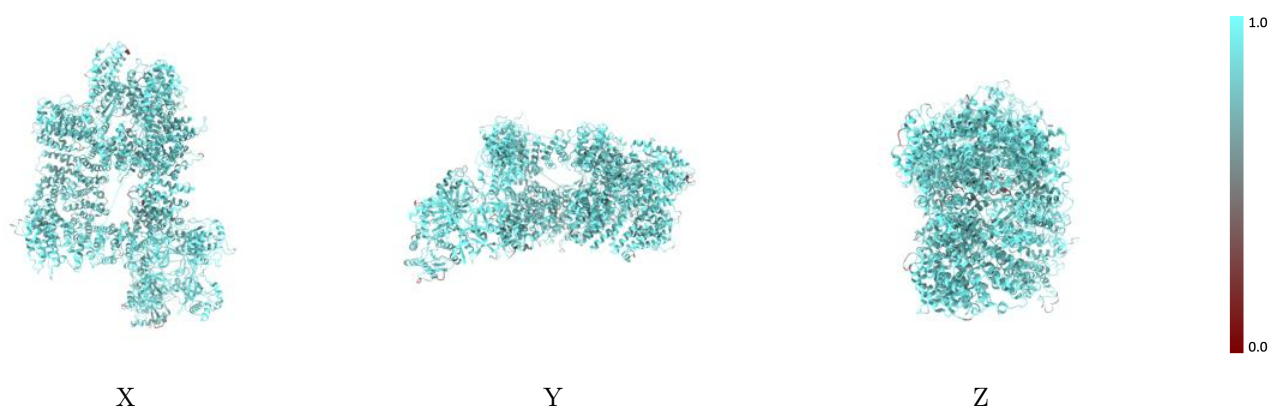
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



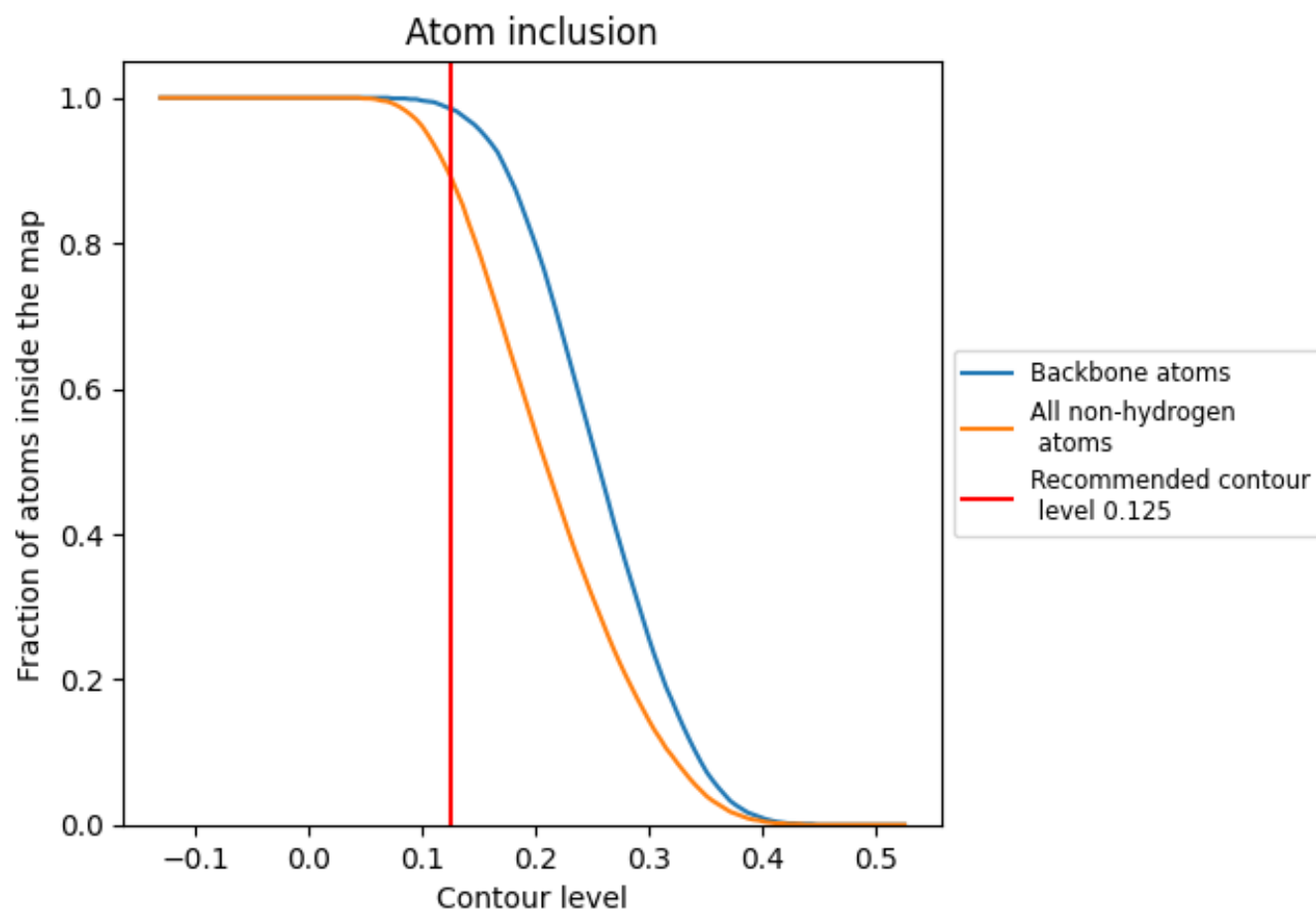
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.3380
A	0.8960	0.3460
B	0.8940	0.3370
C	0.8550	0.2850
D	0.9940	0.3340
E	0.9820	0.3100

